

Synthesis, Molecular Docking and Biological Evaluation of New Quinoline Analogues as Potent Anti-breast cancer and Antibacterial agents

Shrimant V. Rathod^{*,a}, Kailas W. Shinde^{a,b}, Prashant S. Kharkar^c, Chetan P. Shah^d, K.

Aruna^e, Darshana A. Raut^e

^a Department of Chemistry, Bhavan's Somani and Hazarimal College, Mumbai-400007, India

^b Department of Chemistry, Wilson College, Mumbai-400007, India

^c Department of Pharmaceutical Quality Assurance, SPTM, NMIMS, Mumbai-400056, India

^d Department of Pharmaceutical Chemistry, SPTM, NMIMS, Mumbai-400056, India

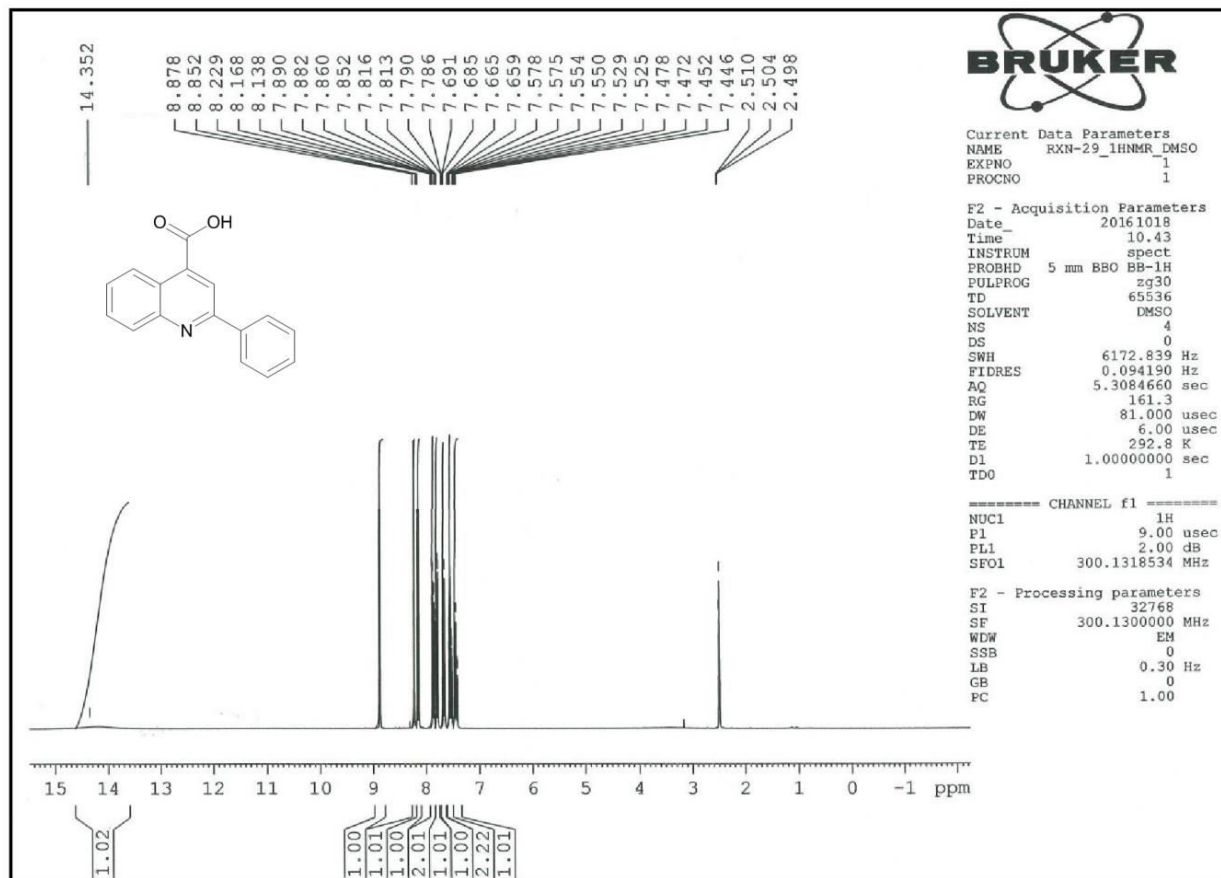
^e Department of Microbiology, Wilson College, Mumbai-400007, India

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2.	¹³ C NMR	13-23
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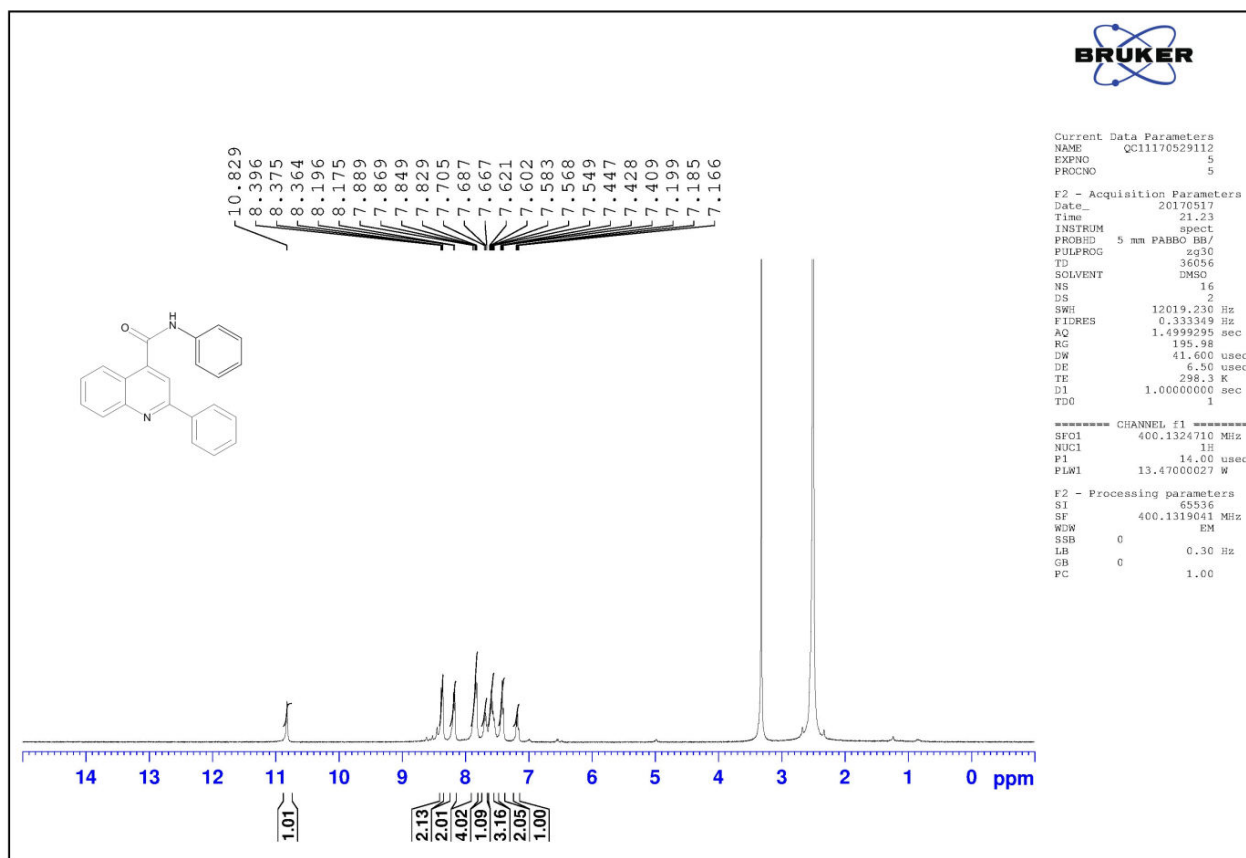
1. ^1H NMR :

^1H NMR of 2-phenylquinoline-4-carboxylic acid (3)



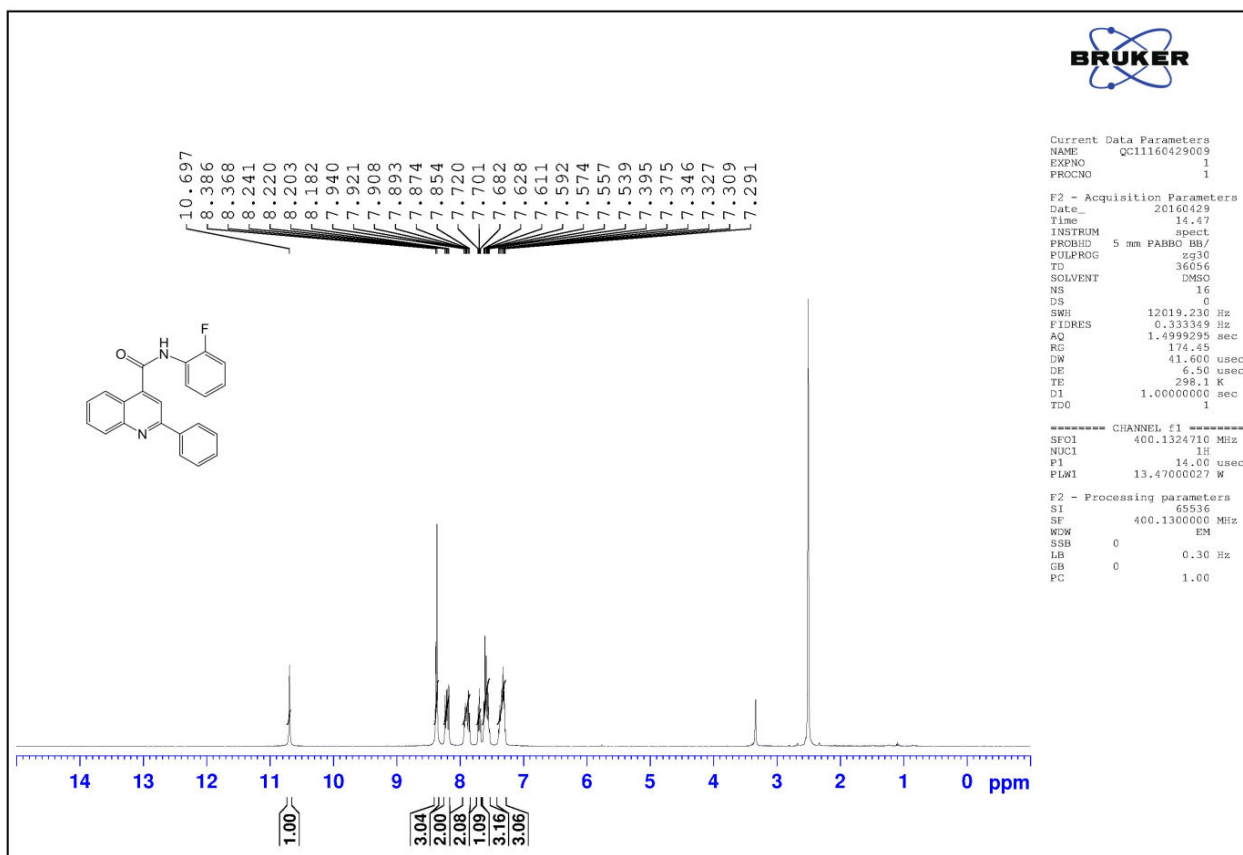
^1H NMR (DMSO- d_6 , 300MHz, δ ppm): 14.35 (brs, 1H), 8.87 (d, $J = 7.8$ Hz, 1H), 8.22 (s, 1H), 8.15 (d, $J = 9.0$ Hz, 1H), 7.85-7.89 (m, 2H), 7.78-7.81 (m, 1H), 7.65-7.69 (m, 1H), 7.52-7.57 (m, 2H), 7.44-7.47 (m, 1H)

¹H NMR of Synthesis of *N,N*-2-diphenylquinoline-4-carboxamide (4a)



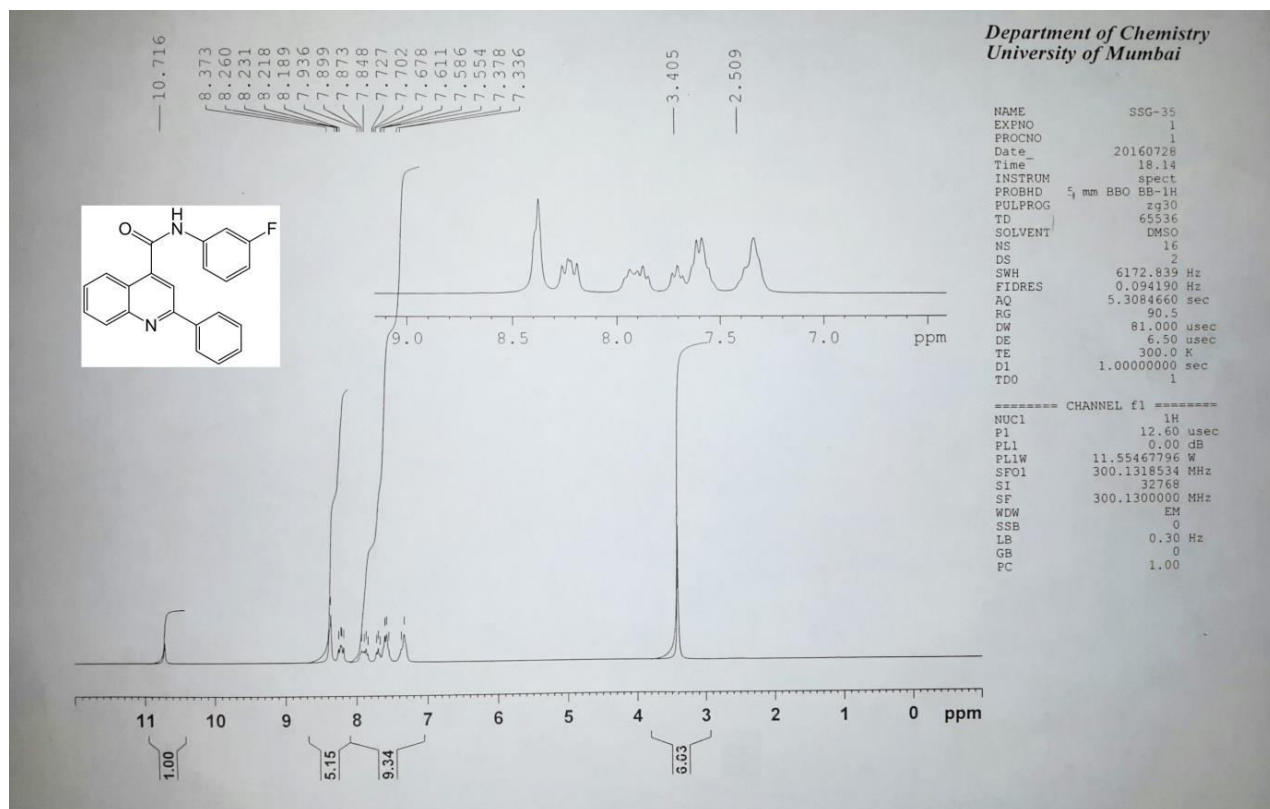
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.82 (s, 1H), 8.37 (t, 2H), 8.18 (d, *J* = 8.4 Hz, 2H), 7.82-7.88 (m, 4H), 7.68 (t, 1H), 7.54-7.62 (m, 3H), 7.42 (t, 2H), 7.18 (t, 1H)

¹H NMR of *N*-(2-fluorophenyl)-2-phenylquinoline-4-carboxamide (**4b**)



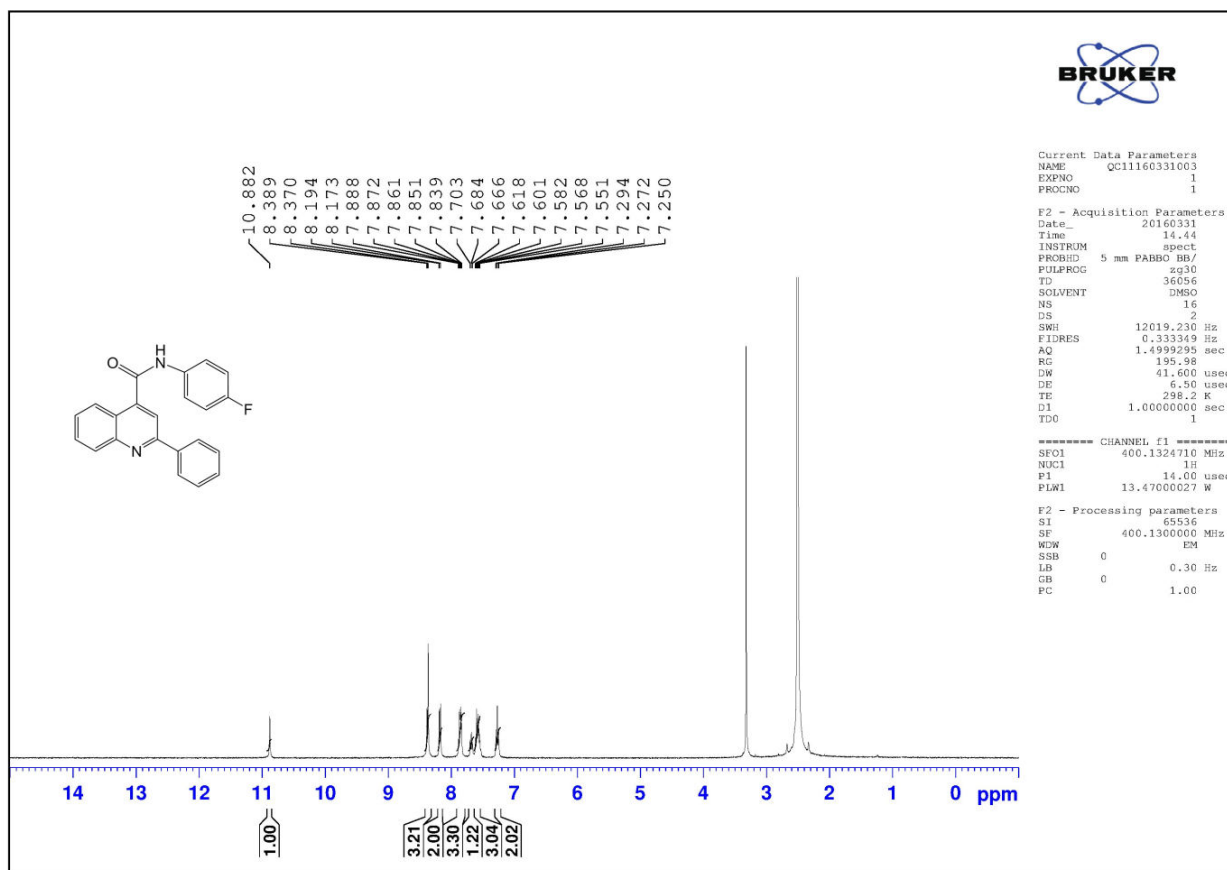
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.69 (s, 1H), 8.37 (d, *J* = 7.2 Hz, 3H), 8.18-8.24 (m, 2H), 7.85-7.94 (m, 2H), 7.70 (t, 1H), 7.53-7.62 (m, 3H), 7.29-7.39 (m, 3H)

¹H NMR of N-(3-fluorophenyl)-2-phenylquinoline-4-carboxamide (4c)



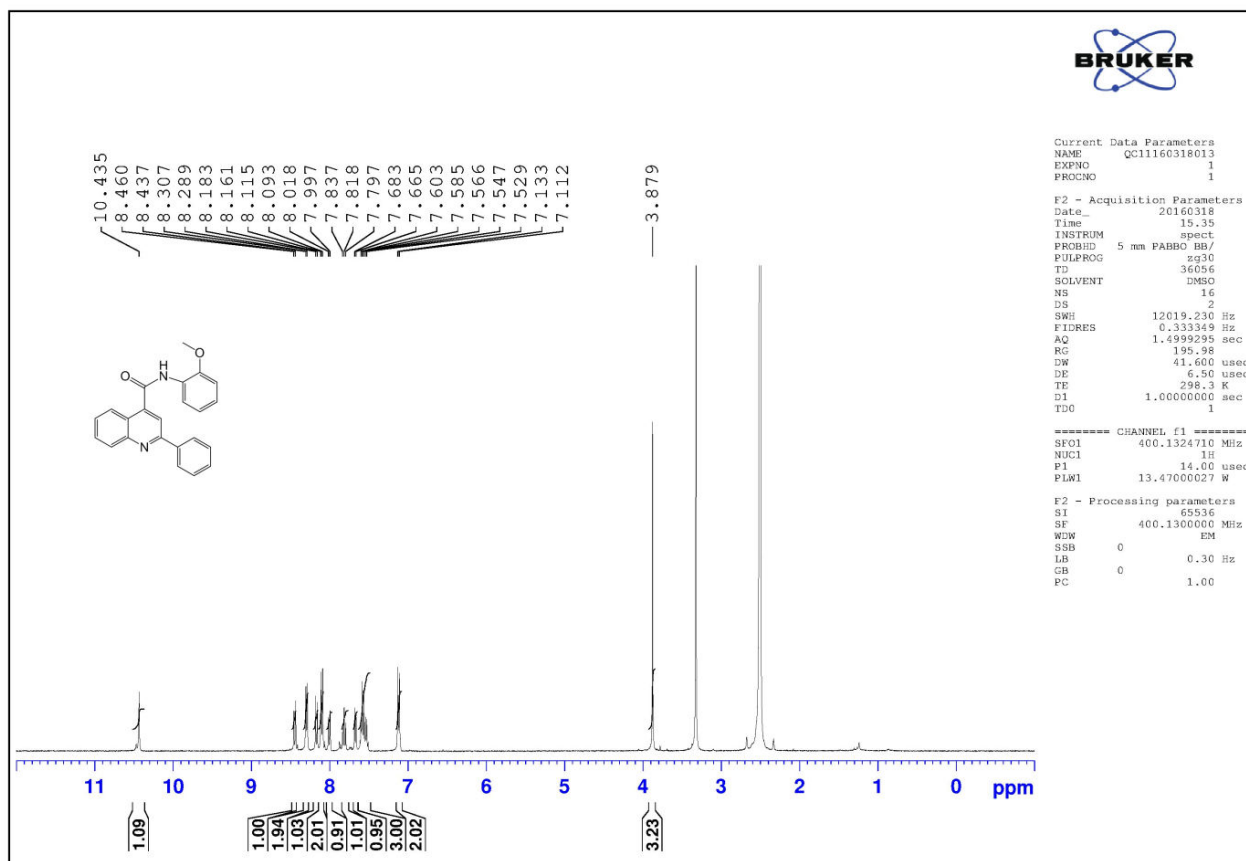
¹H NMR (DMSO-d₆, 300MHz, δ ppm): 10.71 (s, 1H), 8.37 (s, 1H), 8.18-8.26 (m, 4H), 7.84-7.93 (m, 2H), 7.70 (t, 2H), 7.58 (t, 3H), 7.33-7.37 (m, 2H)

¹H NMR of N-(4-fluorophenyl)-2-phenylquinoline-4-carboxamide (4d)



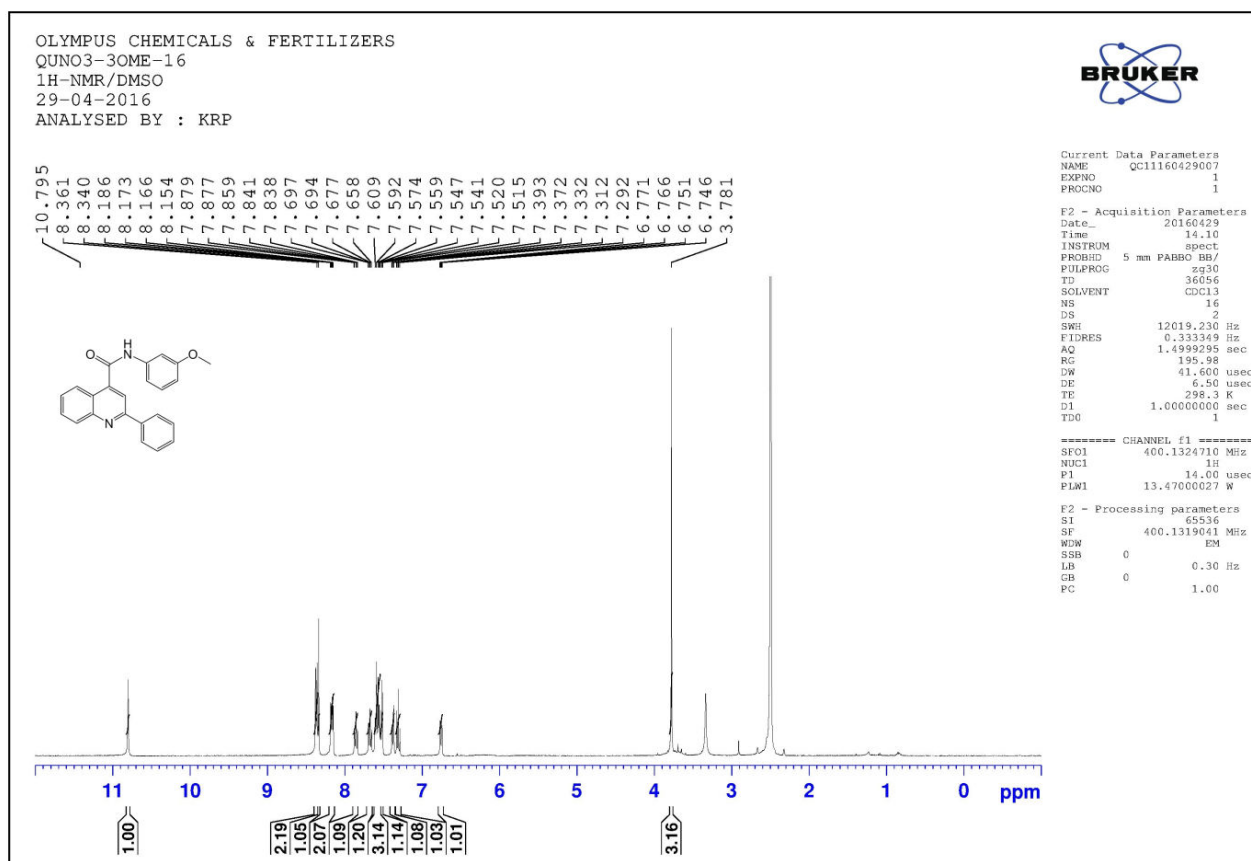
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.88 (s, 1H), 8.38 (d, *J* = 7.6 Hz, 3H), 8.18 (d, *J* = 8.4 Hz, 2H), 7.83-7.88 (m, 3H), 7.68 (t, 1H), 7.55-7.61 (m, 3H), 7.27 (t, 2H)

¹H NMR of *N*-(2-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4e)



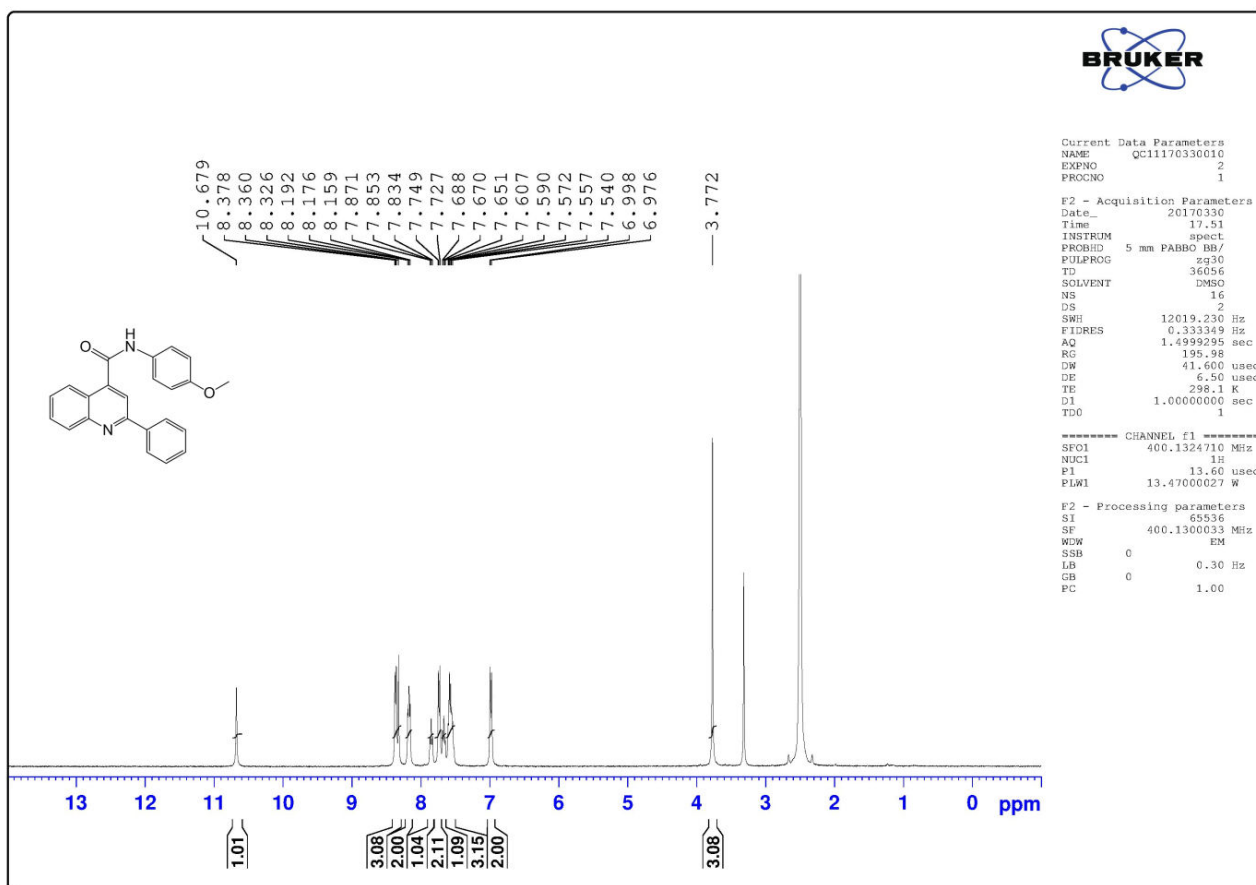
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.43 (s, 1H), 8.45 (d, *J* = 9.2 Hz, 1H), 8.29 (d, *J* = 7.2 Hz, 2H), 8.17 (d, *J* = 8.8 Hz, 1H), 8.10 (d, *J* = 8.8 Hz, 2H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.81 (t, 1H), 7.67 (d, *J* = 7.2 Hz, 1H), 7.52-7.60 (m, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 3.88 (s, 3H)

¹H NMR of *N*-(3-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4f)



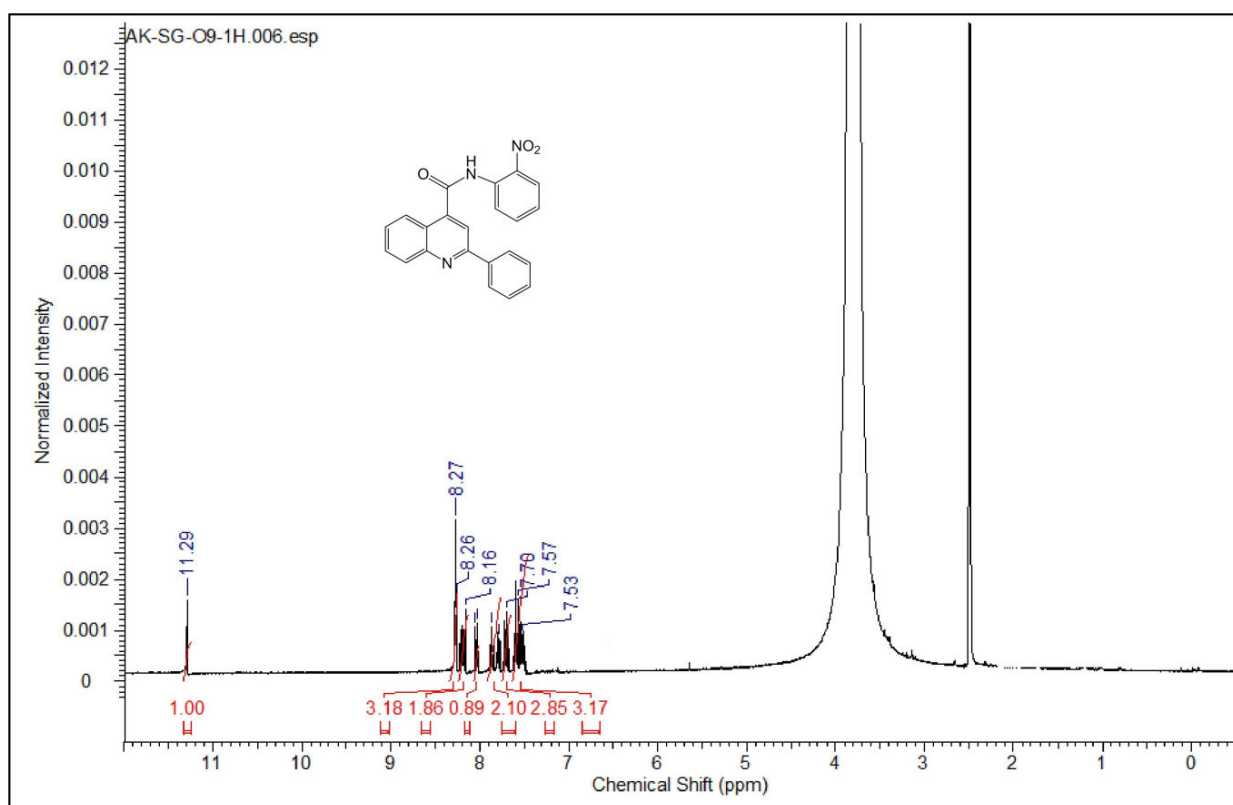
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.79 (s, 1H), 8.35 (d, *J* = 8.4 Hz, 3H), 8.15-8.18 (m, 2H), 7.83-7.87 (m, 1H), 7.65-7.69 (m, 1H), 7.51-7.60 (m, 4H), 7.38 (d, *J* = 8.4 Hz, 1H), 7.31 (t, 1H), 6.74-6.77 (m, 1H), 3.78 (s, 3H)

¹H NMR of *N*-(4-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4g)



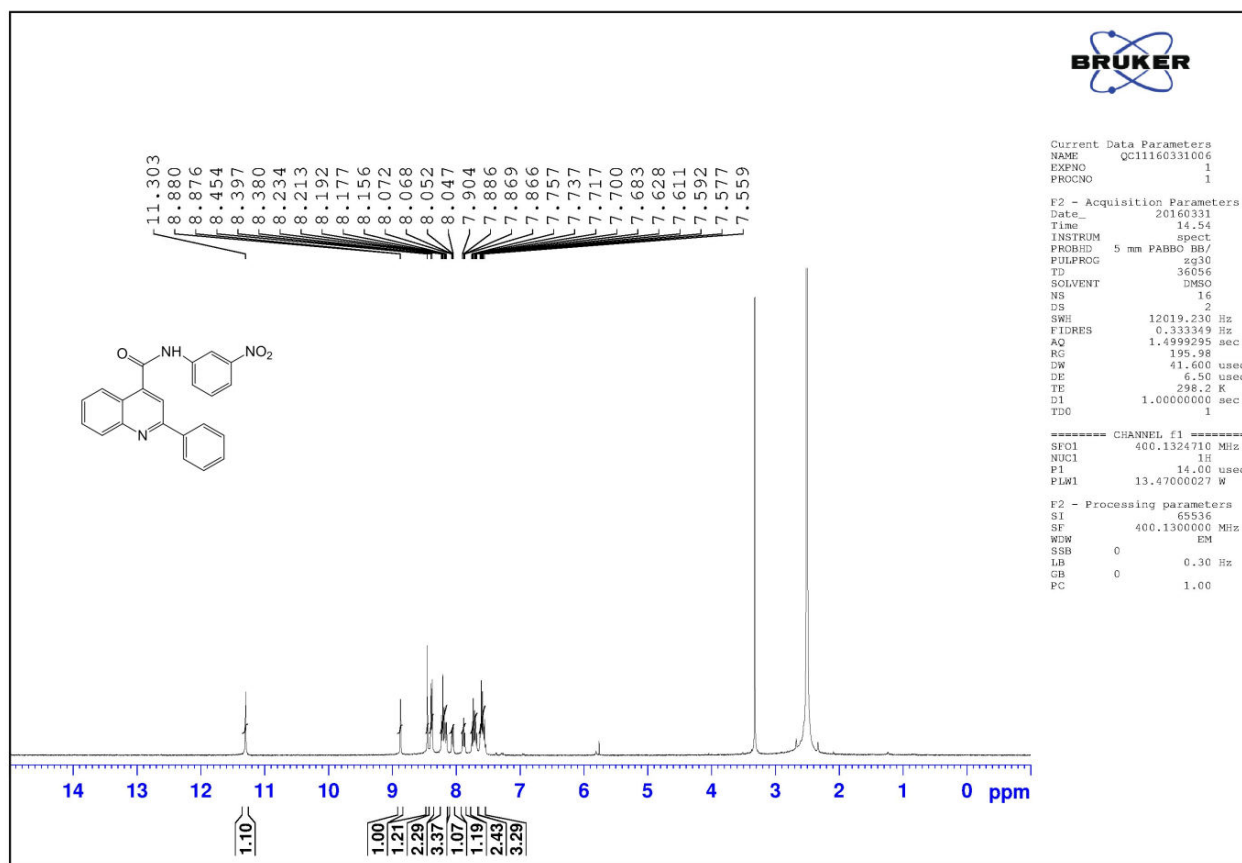
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 10.67 (s, 1H), 8.37 (d, *J* = 7.2 Hz, 2H), 8.32 (s, 1H), 8.17 (t, 2H), 7.85 (t, 1H), 7.73 (d, *J* = 8.8 Hz, 2H), 7.67 (t, 1H), 7.54-7.60 (m, 3H), 6.98 (d, *J* = 8.8 Hz, 2H), 3.77 (s, 3H)

¹H NMR of N-(2-nitrophenyl)-2-phenylquinoline-4-carboxamide (4h)



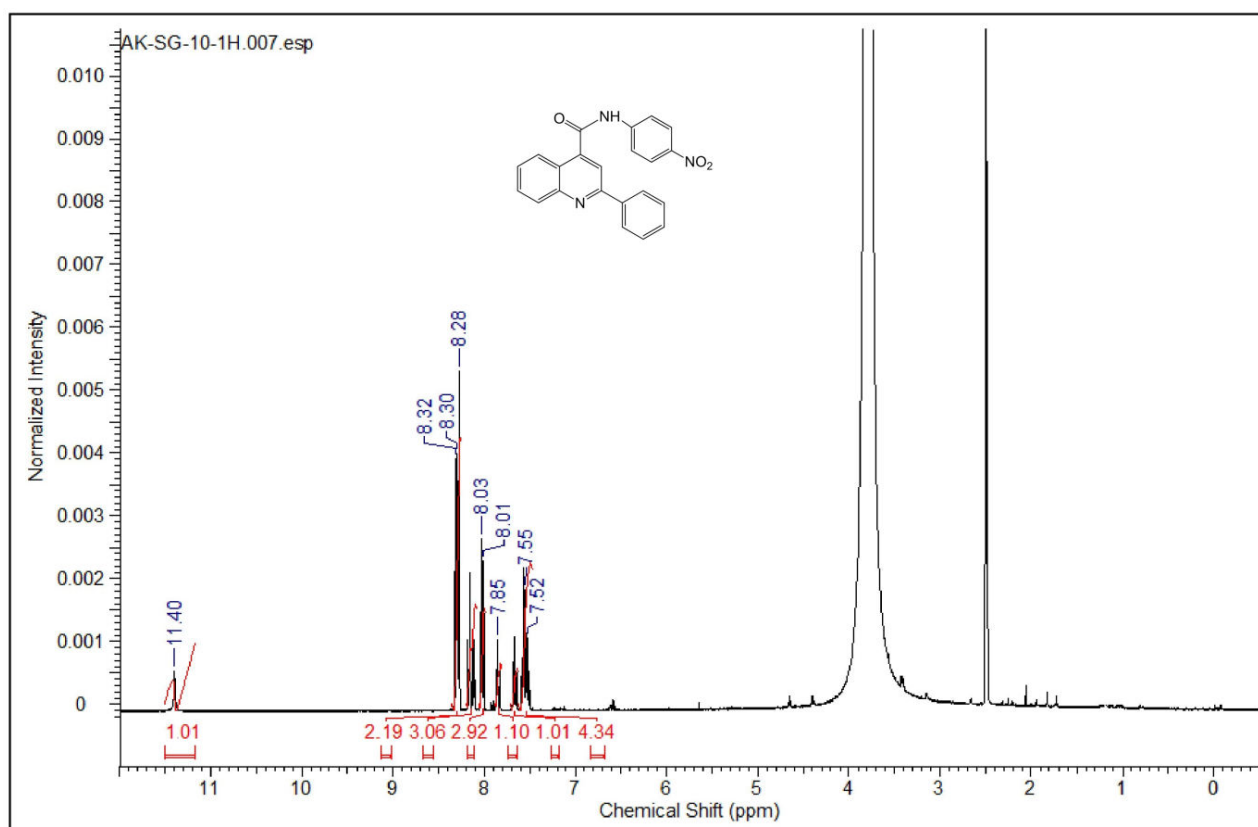
¹H NMR (DMSO-d₆, 400MHz, δ ppm): 11.29 (s, 1H), 8.27 (m, 3H), 8.26 (m, 2H), 8.16 (m, 1H), 7.70 (m, 2H), 7.57 (m, 3H), 7.53 (m, 3H)

¹H NMR of *N*-(3-nitrophenyl)-2-phenylquinoline-4-carboxamide (4i)



¹H NMR (DMSO-d₆, 400MHz, δ ppm): 11.30 (s, 1H), 8.88 (d, *J* = 1.6 Hz, 1H), 8.45 (s, 1H), 8.39 (d, *J* = 6.8 Hz, 2H), 8.15-8.23 (m, 3H), 8.04-8.07 (m, 1H), 7.86-7.90 (m, 1H), 7.68-7.75 (m, 2H), 7.55-7.62 (m, 3H)

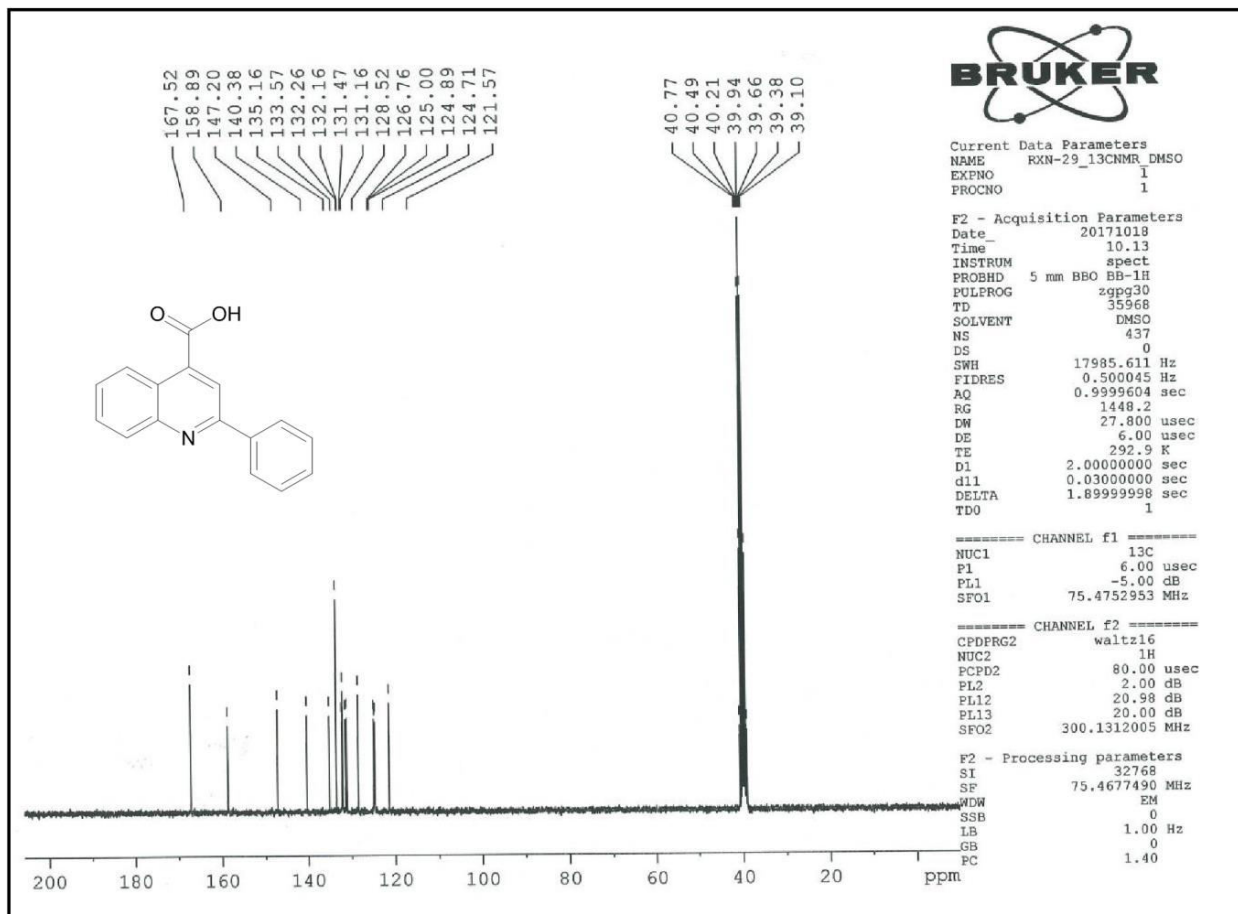
¹H NMR of N-(4-nitrophenyl)-2-phenylquinoline-4-carboxamide (4j)



¹H NMR (DMSO-d₆, 400MHz, δ ppm): 11.40 (s, 1H), 8.31 (m, 2H), 8.28 (m, 3H), 8.02 (d, *J* = 8.0 Hz, 3H), 7.85 (m, 1H), 7.55 (m, 1H), 7.52 (m, 4H)

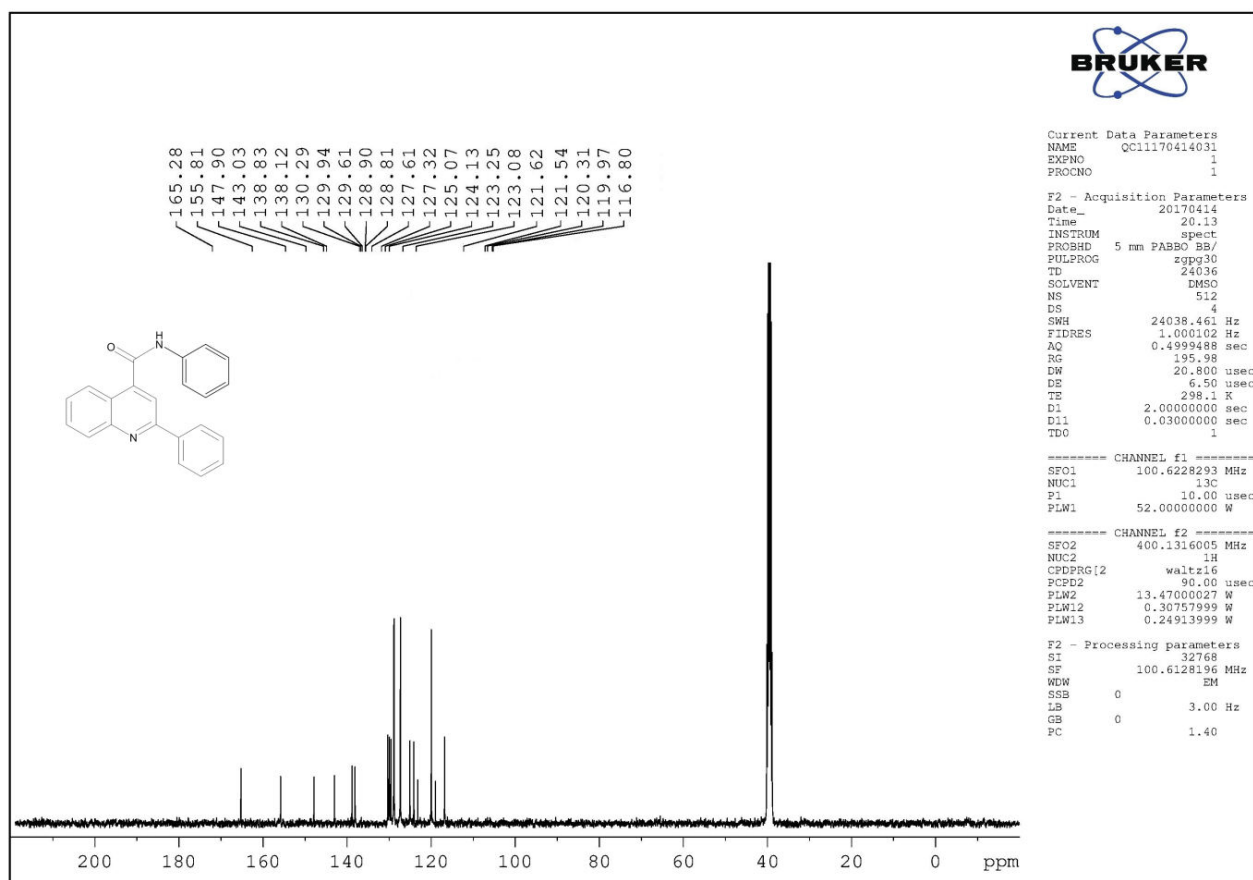
2. ^{13}C NMR :

^{13}C NMR of 2-phenylquinoline-4-carboxylic acid (3)



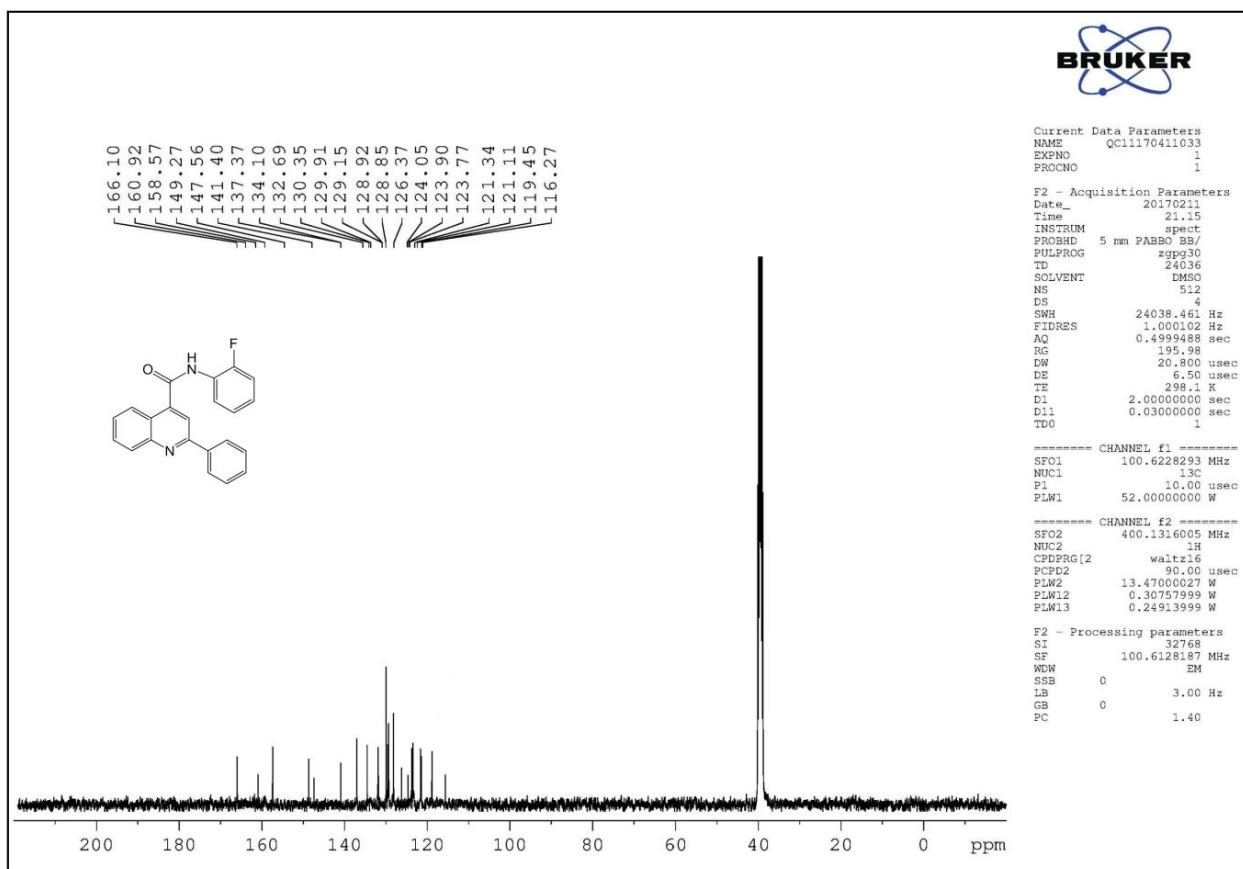
^{13}C NMR (DMSO- d_6 , 300MHz, δ ppm): 167.52, 158.89, 147.20, 140.38, 135.16, 133.57, 132.26, 132.16, 131.47, 131.16, 128.52, 126.76, 125.00, 124.89, 124.71, 121.57

¹³C NMR of Synthesis of *N,N*-2-diphenylquinoline-4-carboxamide (4a)



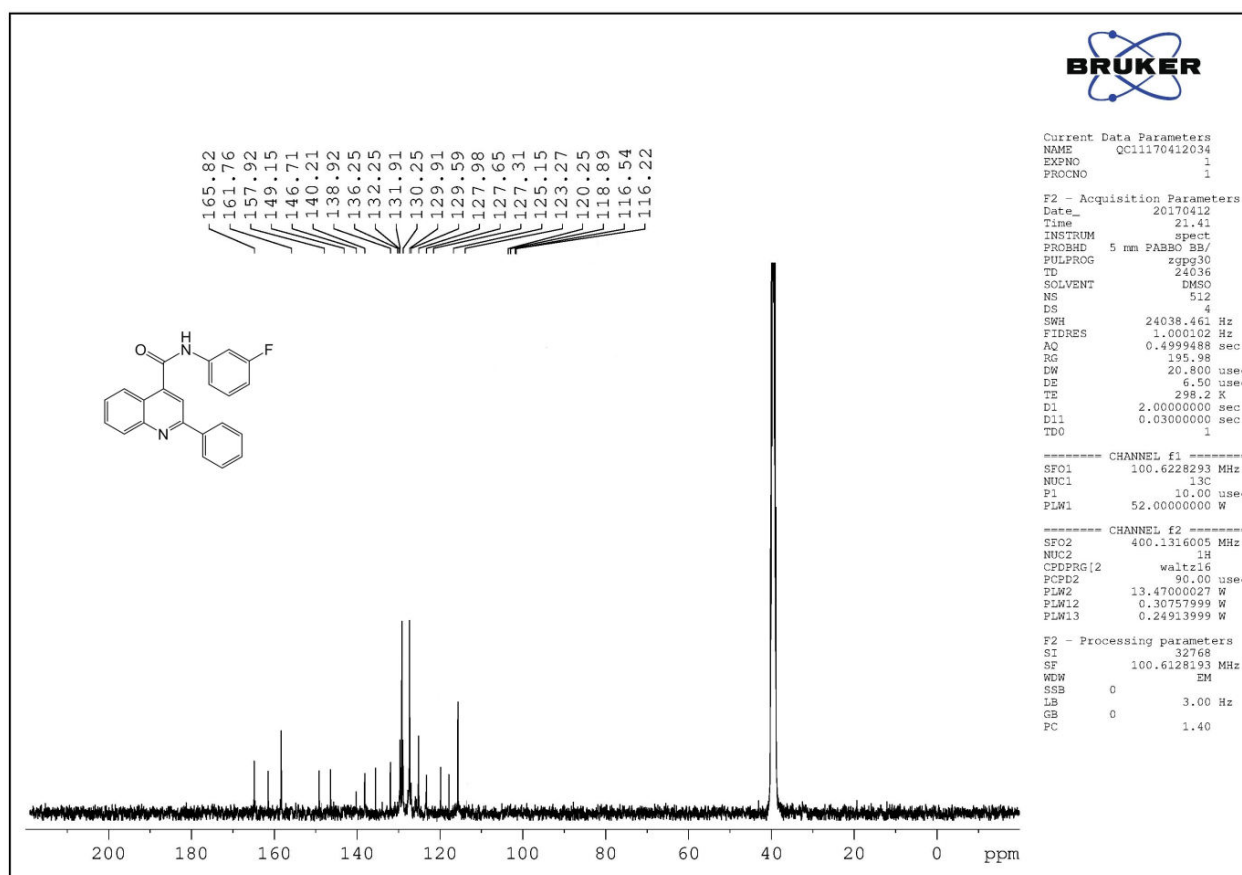
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.28, 155.81, 147.90, 143.03, 138.83, 138.12, 130.29, 129.94, 129.61, 128.90, 128.81, 127.61, 127.32, 125.07, 124.13, 123.25, 123.08, 121.62, 121.54, 120.31, 119.97, 116.80

¹³C NMR of *N*-(2-fluorophenyl)-2-phenylquinoline-4-carboxamide (**4b**)



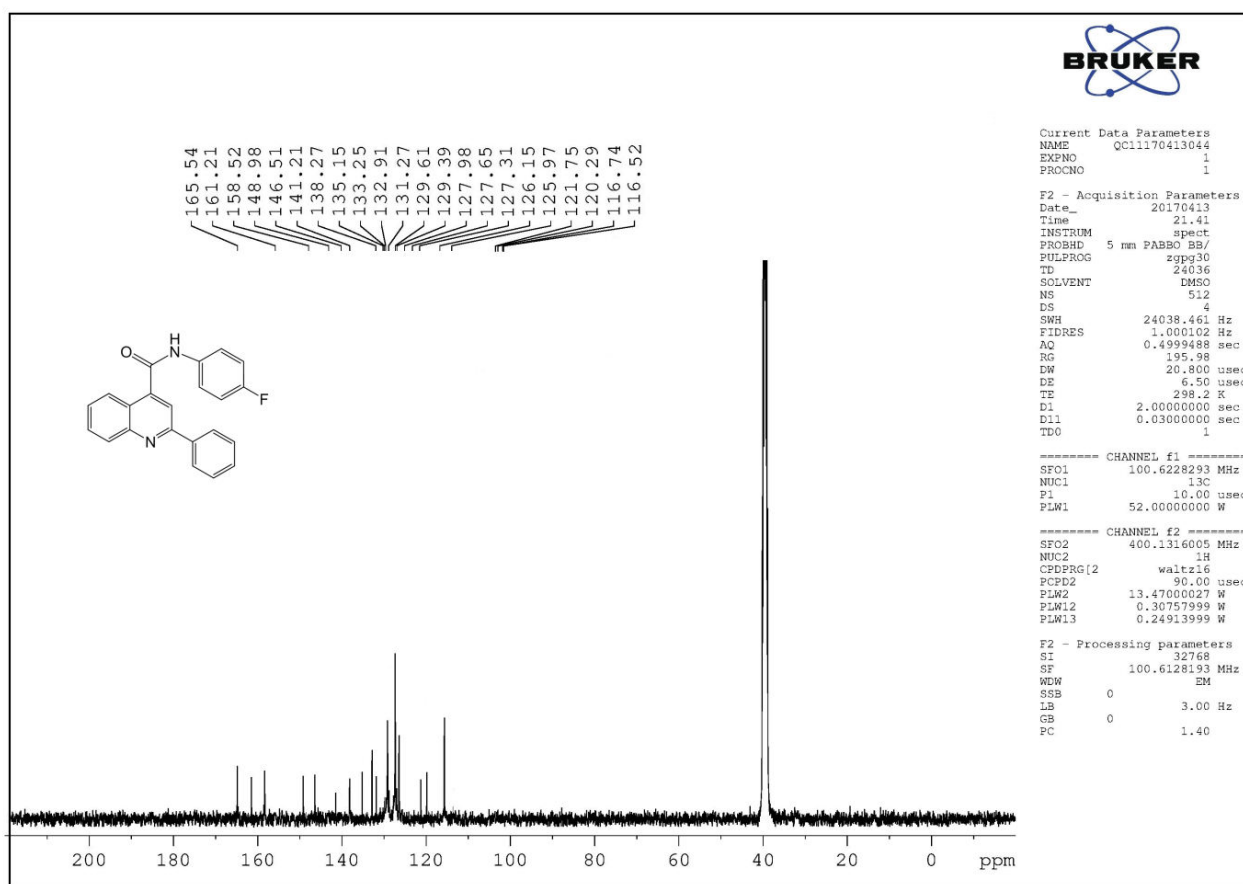
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 166.10, 160.92, 158.57, 149.27, 147.56, 141.40, 137.37, 134.10, 132.69, 130.35, 129.91, 129.15, 128.92, 128.85, 126.37, 124.05, 123.90, 123.77, 121.34, 121.11, 119.45, 116.27

¹³C NMR of *N*-(3-fluorophenyl)-2-phenylquinoline-4-carboxamide (**4c**)



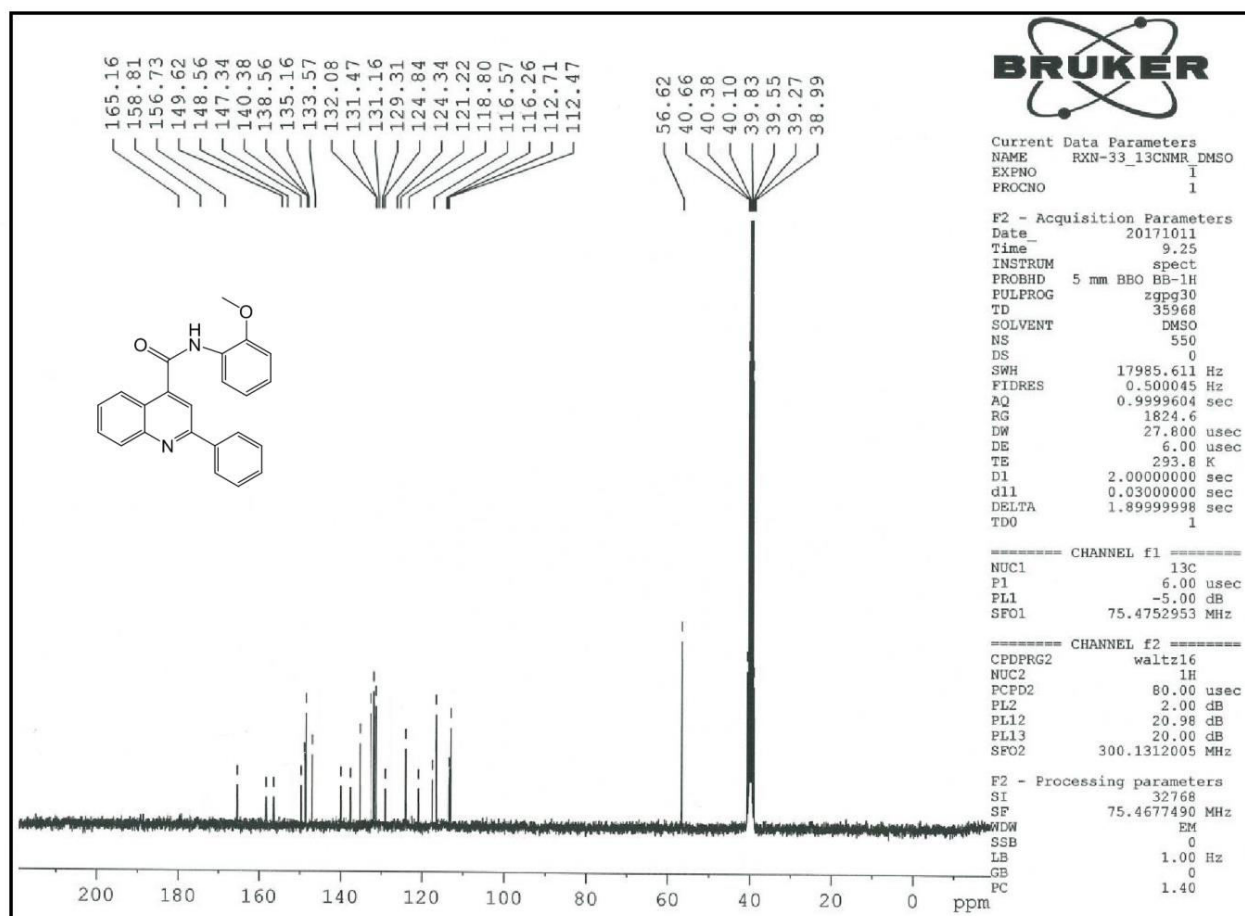
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.82, 161.76, 157.92, 149.15, 146.71, 140.21, 138.92, 136.25, 132.25, 131.91, 130.25, 129.91, 129.59, 127.98, 127.65, 127.31, 125.15, 123.27, 120.25, 118.89, 116.54, 116.22

¹³C NMR of *N*-(4-fluorophenyl)-2-phenylquinoline-4-carboxamide (4d)



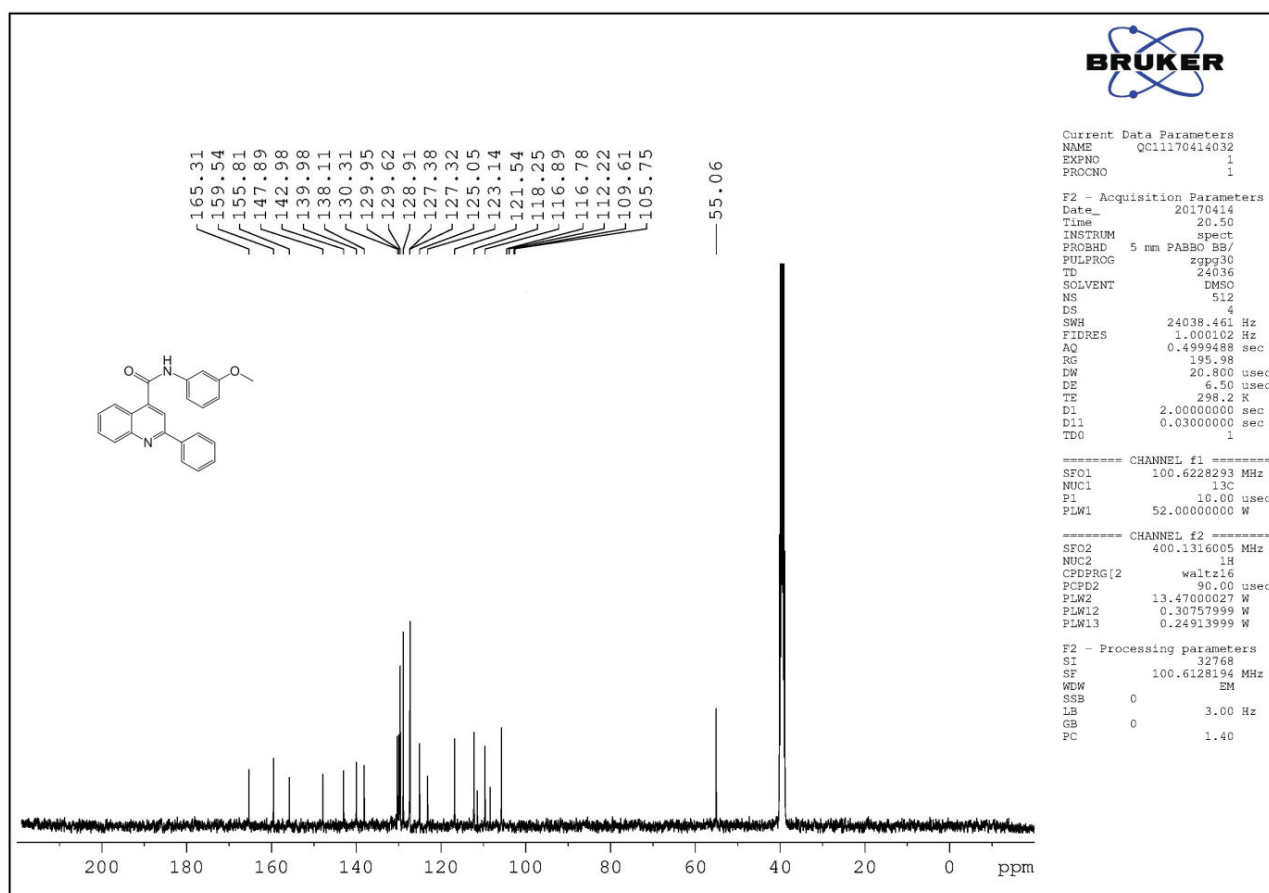
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.54, 161.21, 158.52, 148.98, 146.51, 141.21, 138.27, 135.15, 133.25, 132.91, 131.27, 129.61, 129.39, 127.98, 127.65, 127.31, 126.15, 125.97, 121.75, 120.29, 116.74, 116.52

¹³C NMR of *N*-(2-methoxyphenyl)-2-phenylquinoline-4-carboxamide (*4e*)



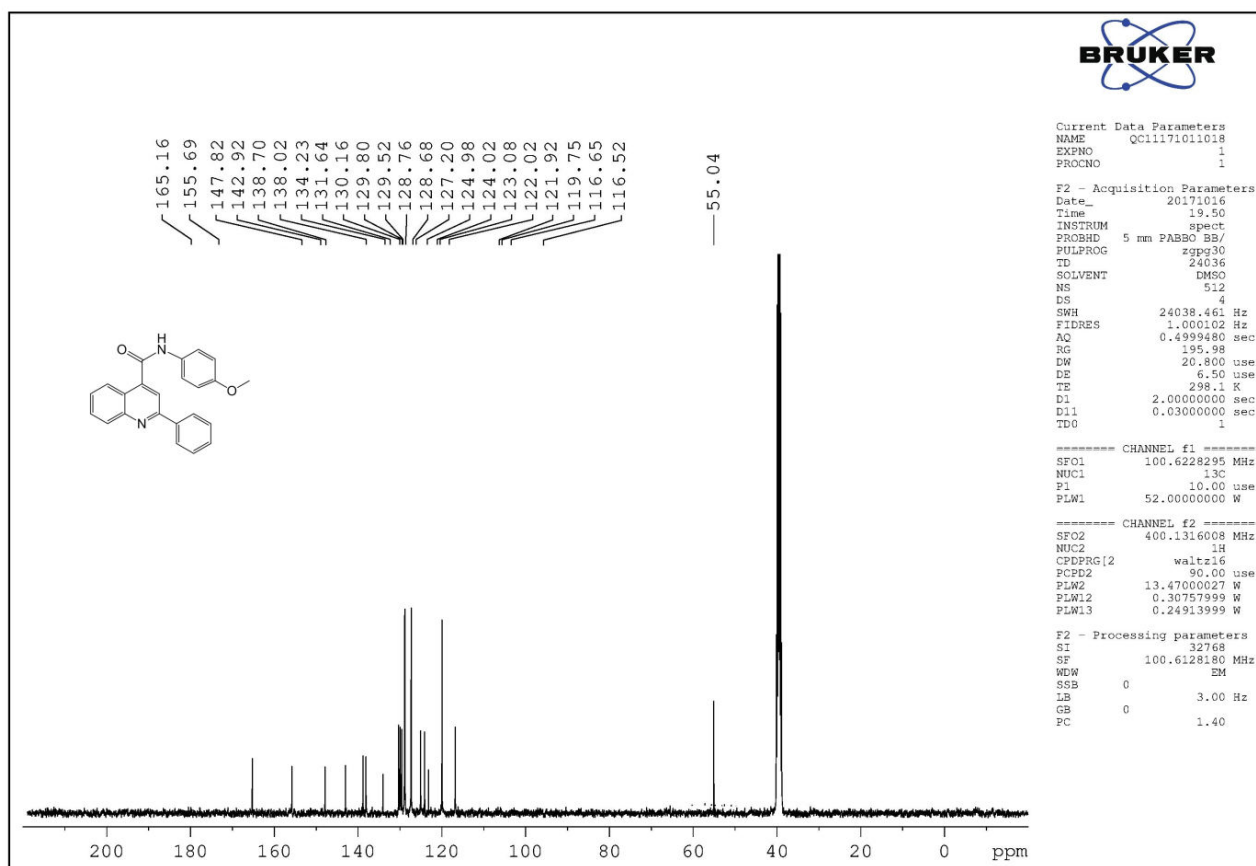
¹³C NMR (DMSO-d₆, 75MHz, δ ppm): 165.16, 158.81, 156.73, 149.62, 148.56, 147.34, 140.38, 138.56, 135.16, 133.57, 132.08, 131.47, 131.16, 129.31, 124.84, 124.34, 121.22, 118.80, 116.57, 116.26, 112.71, 112.47, 56.62

¹³C NMR of *N*-(3-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4f)



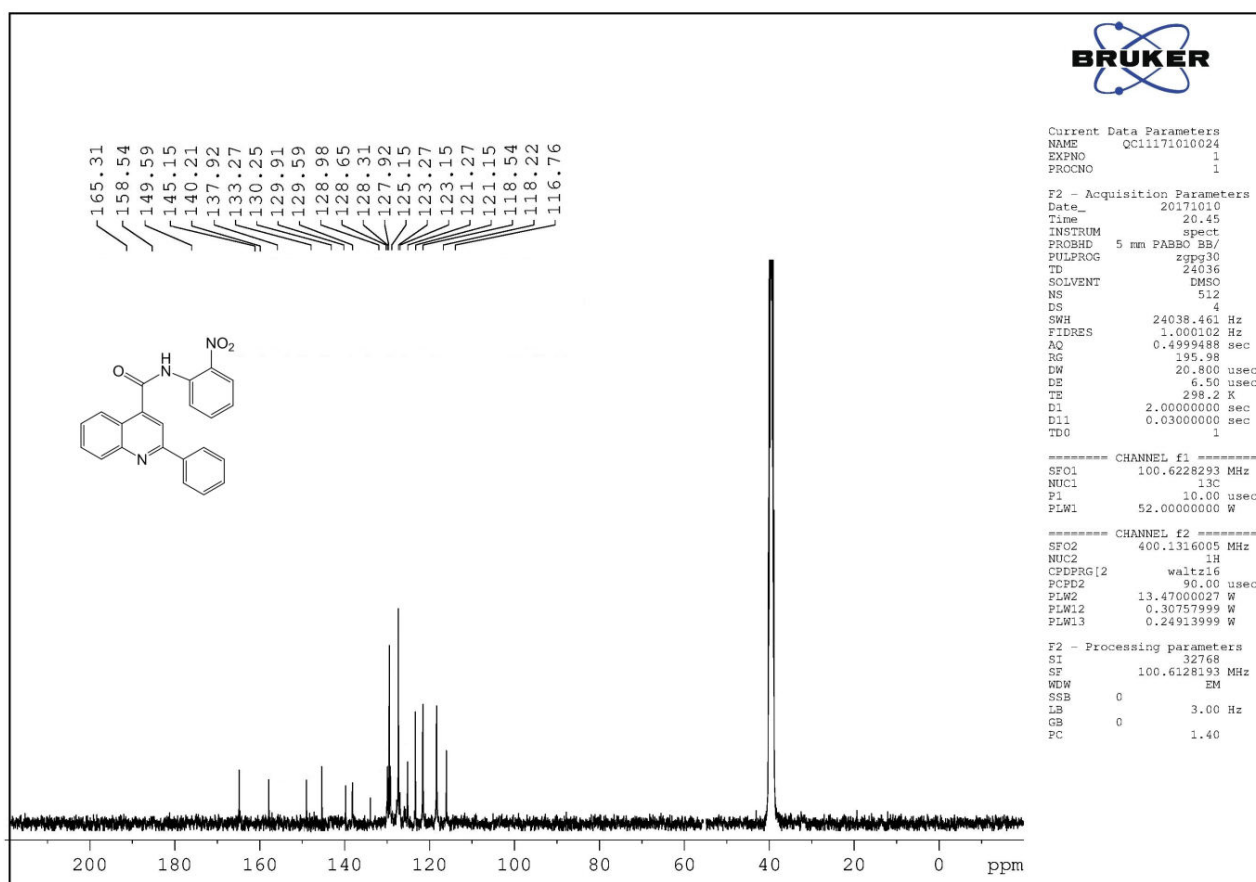
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.31, 159.54, 155.81, 147.89, 142.98, 139.98, 138.11, 130.31, 129.95, 129.62, 128.91, 127.38, 127.32, 125.05, 123.14, 121.54, 118.25, 116.89, 116.78, 112.22, 109.61, 105.75, 55.06

¹³C NMR of *N*-(4-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4g)



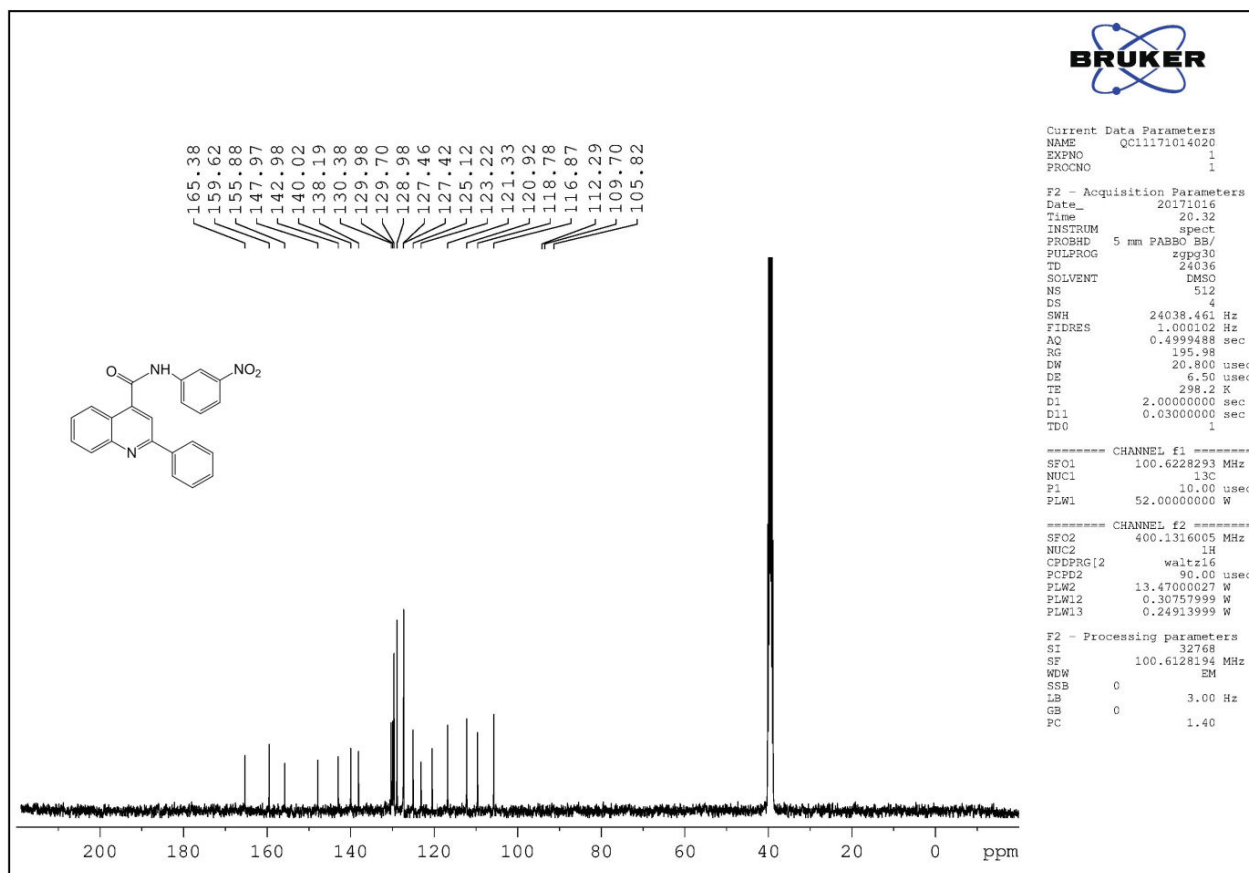
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.16, 155.69, 147.82, 142.92, 138.70, 138.02, 134.23, 131.64, 130.16, 129.80, 129.52, 128.76, 128.68, 127.20, 124.98, 124.02, 123.08, 122.02, 121.92, 119.75, 116.65, 116.52, 55.04

¹³C NMR of *N*-(2-nitrophenyl)-2-phenylquinoline-4-carboxamide (4h)



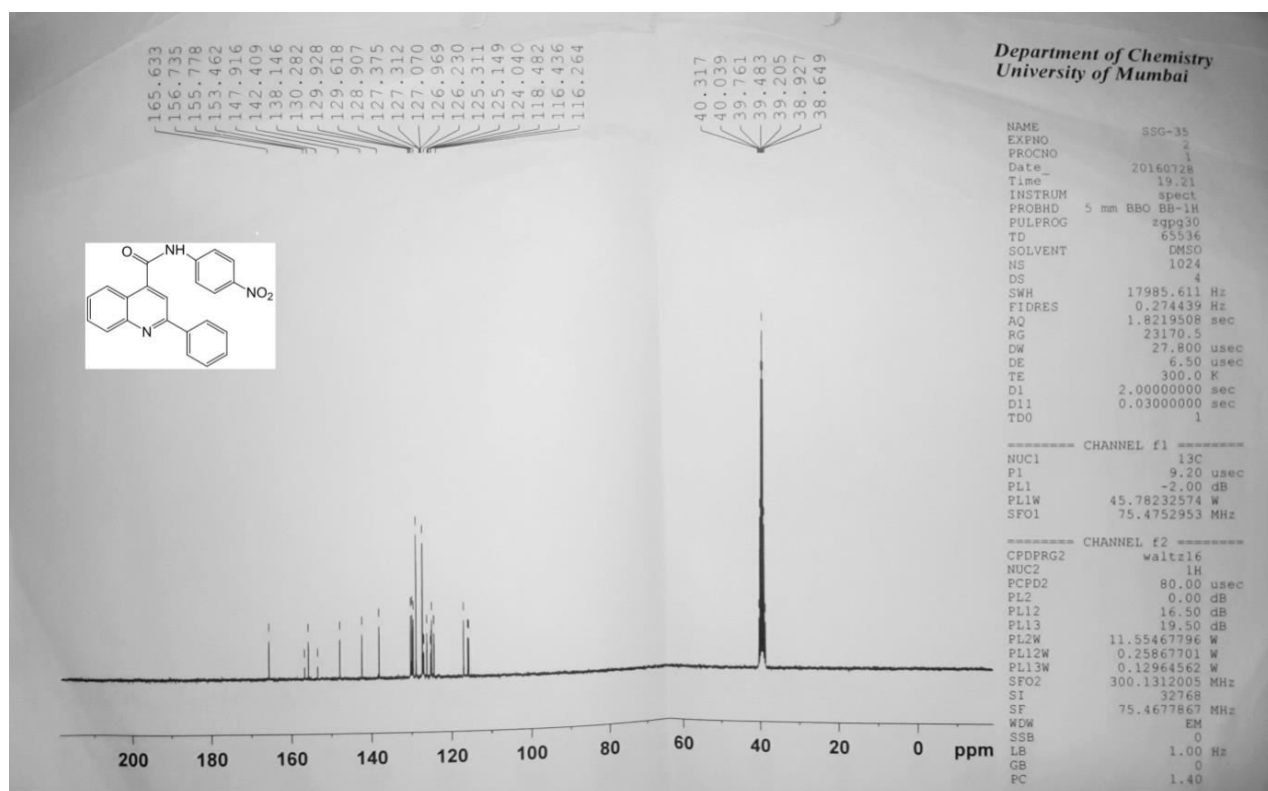
¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.31, 158.54, 149.59, 145.15, 140.21, 137.92, 133.27, 130.25, 129.91, 129.59, 128.98, 128.65, 128.31, 127.92, 125.15, 123.27, 123.15, 121.27, 121.15, 118.54, 118.22, 116.76

¹³C NMR of *N*-(3-nitrophenyl)-2-phenylquinoline-4-carboxamide (4i)



¹³C NMR (DMSO-d₆, 100MHz, δ ppm): 165.38, 159.62, 155.88, 147.97, 142.98, 140.02, 138.19, 130.38, 129.98, 129.70, 128.98, 127.46, 127.42, 125.12, 123.22, 121.33, 120.92, 118.78, 116.87, 112.29, 109.70, 105.82

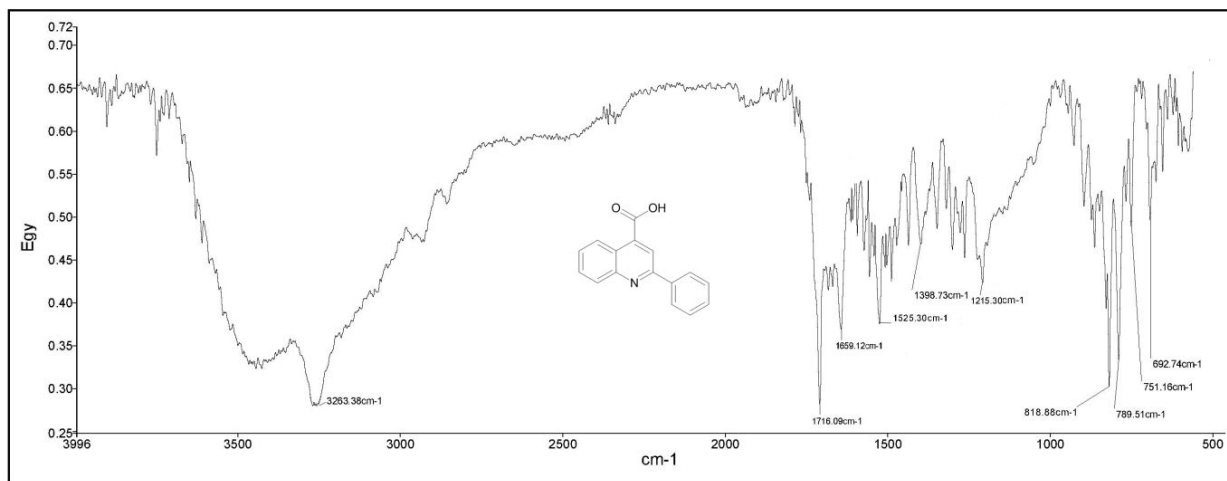
¹³C NMR of N-(4-nitrophenyl)-2-phenylquinoline-4-carboxamide (4j)



¹³C NMR (DMSO-d₆, 75MHz, δ ppm): 165.63, 156.73, 155.77, 153.46, 147.91, 142.40, 138.14, 130.28, 129.92, 129.61, 128.90, 127.37, 127.31, 127.07, 126.96, 126.23, 125.31, 125.14, 124.04, 118.48, 116.43, 116.26

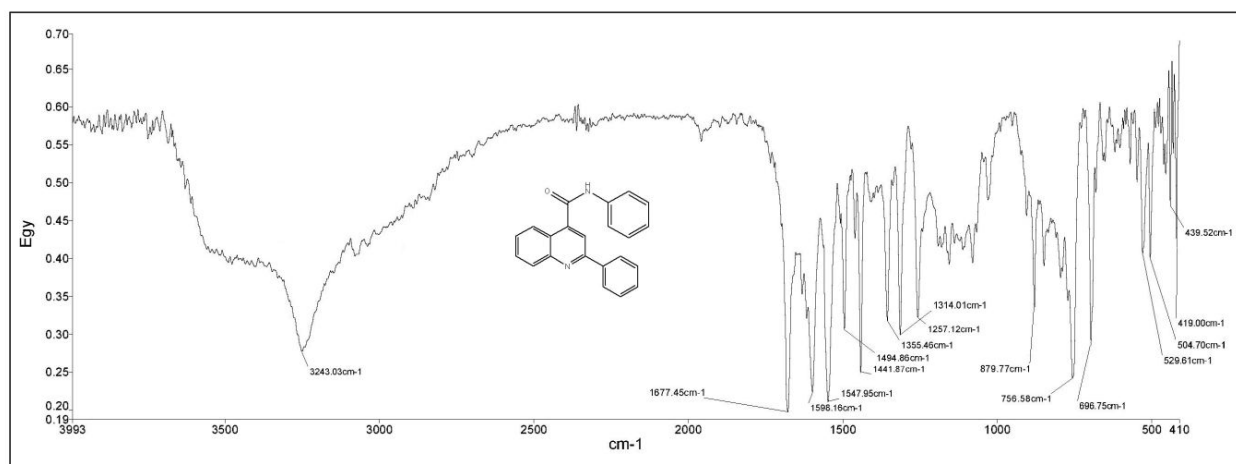
3. IR :

IR of 2-phenylquinoline-4-carboxylic acid (3)



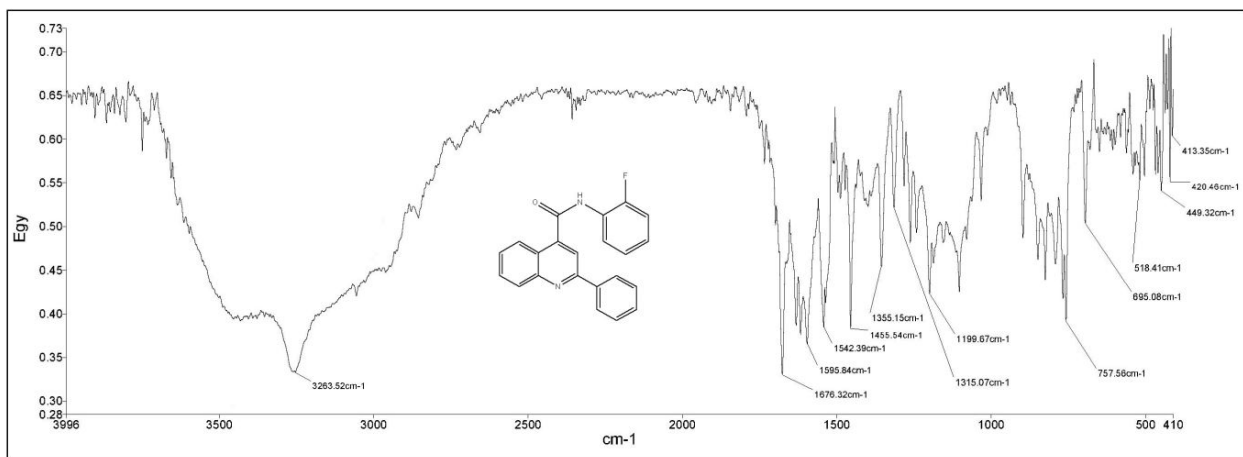
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3263, 1716, 1659, 1525, 1398, 1215, 818, 751, 692

IR of Synthesis of N,N-2-diphenylquinoline-4-carboxamide (4a)



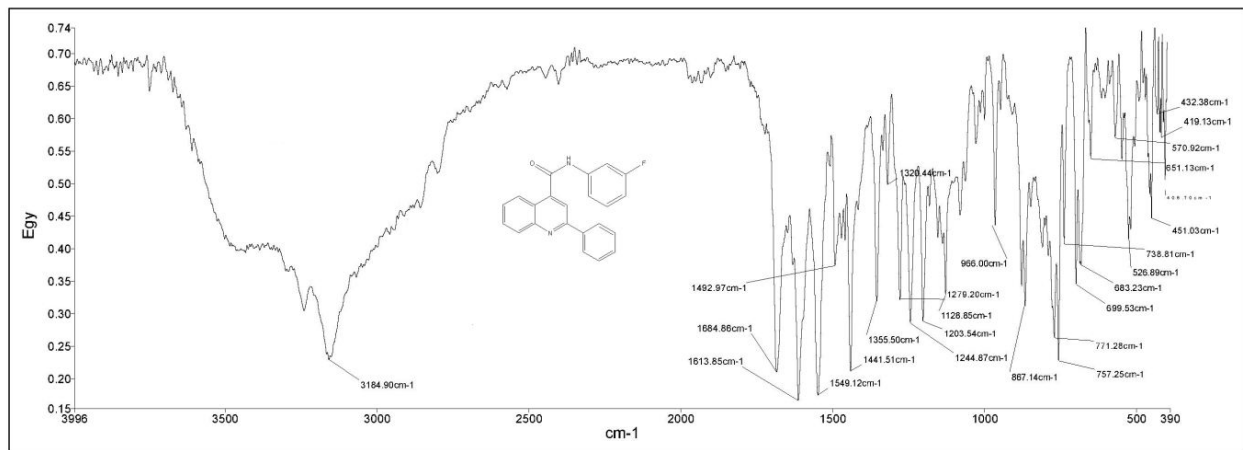
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3243, 1677, 1598, 1547, 1355, 1257, 879, 756, 696

IR of *N*-(2-fluorophenyl)-2-phenylquinoline-4-carboxamide (4b)



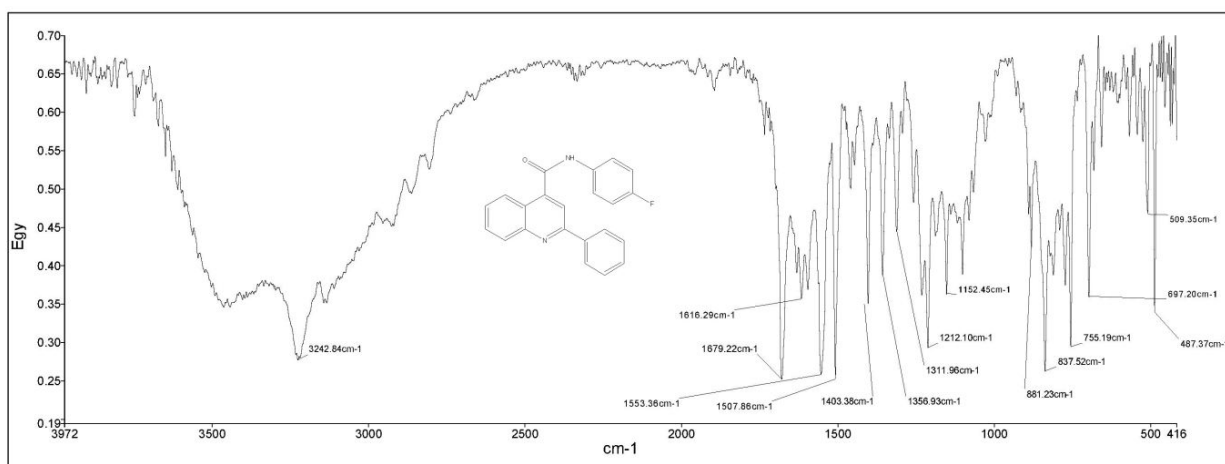
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3263, 1676, 1595, 1542, 1355, 1199, 757, 695

IR of *N*-(3-fluorophenyl)-2-phenylquinoline-4-carboxamide (4c)



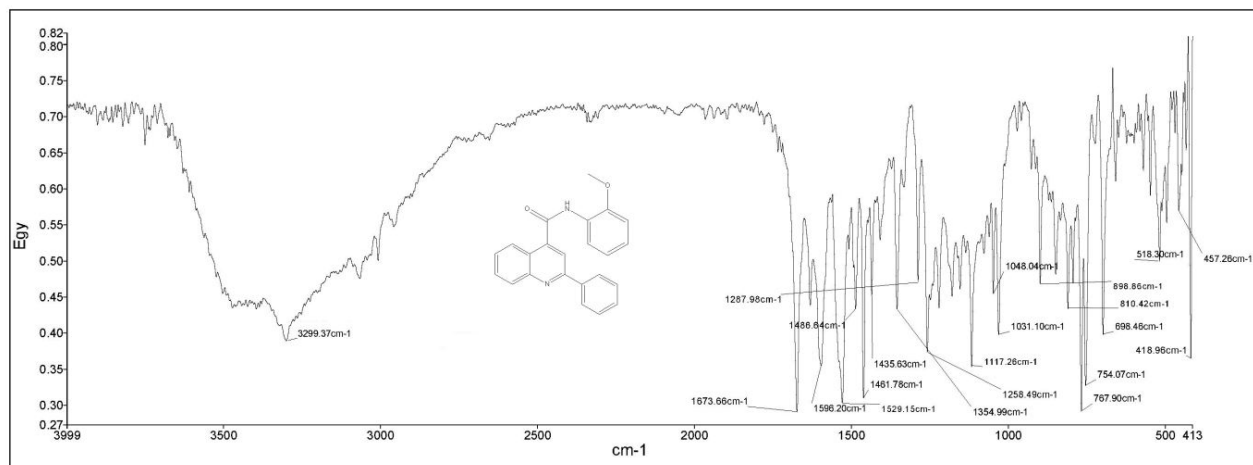
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3184, 1684, 1613, 1549, 1355, 1244, 1128, 867, 757, 699

IR of *N*-(4-fluorophenyl)-2-phenylquinoline-4-carboxamide (4d)



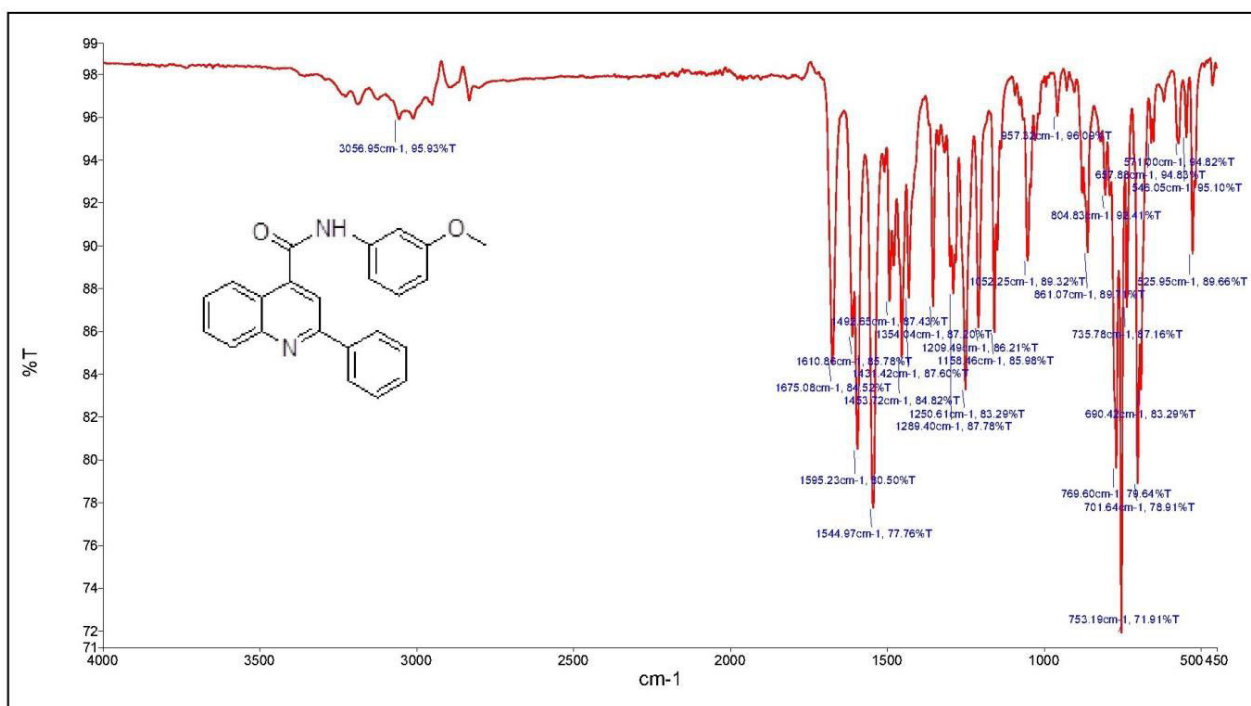
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3242, 1679, 1616, 1553, 1356, 1212, 1152, 837, 755, 697

IR of *N*-(2-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4e)



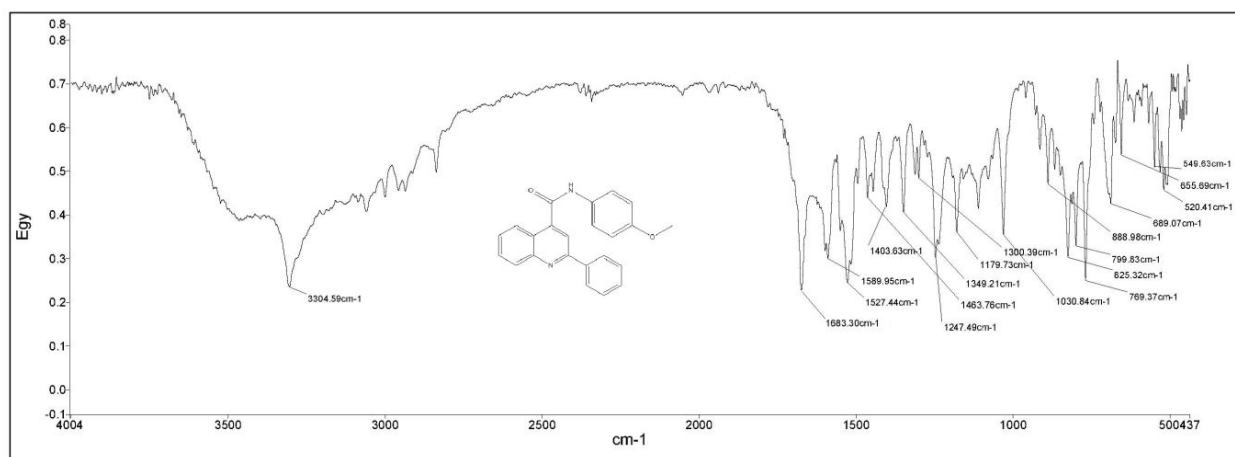
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3299, 1673, 1596, 1529, 1354, 1258, 1117, 1031, 810, 754, 698

IR of *N*-(3-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4f)



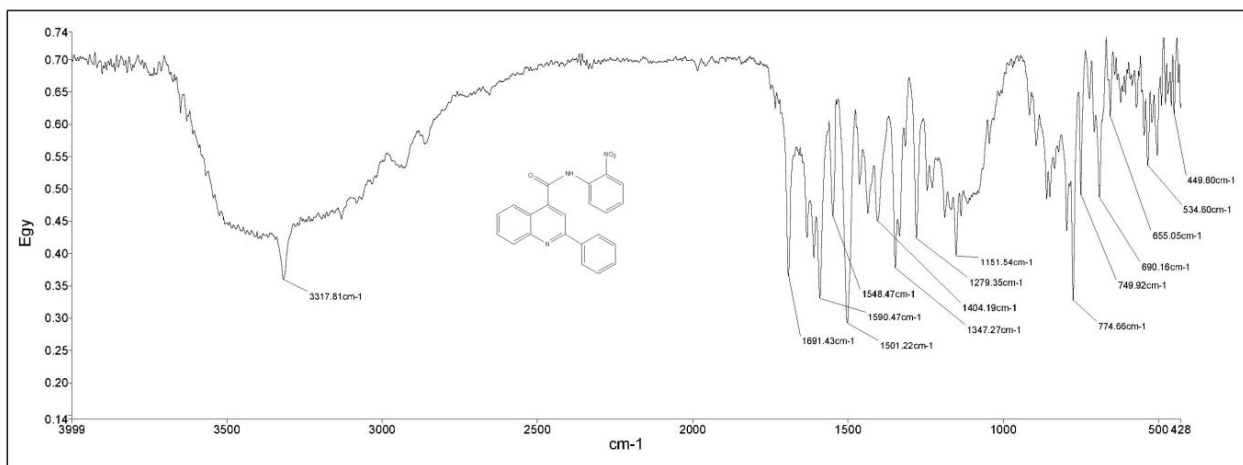
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3056, 1675, 1610, 1544, 1354, 1250, 1158, 861, 753, 690

IR of *N*-(4-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4g)



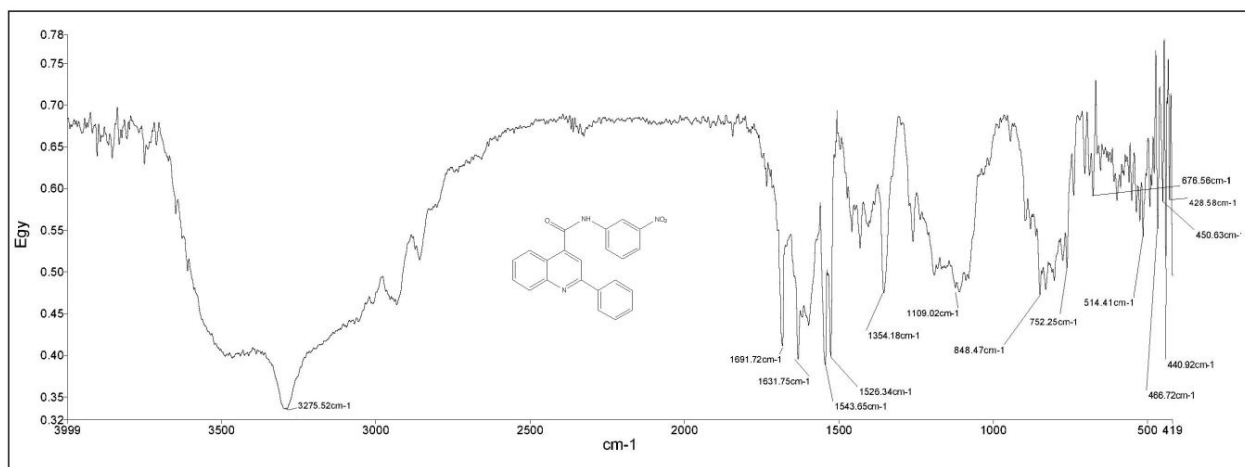
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3304, 1683, 1589, 1527, 1349, 1247, 1179, 1030, 825, 769, 689

IR of *N*-(2-nitrophenyl)-2-phenylquinoline-4-carboxamide (4h)



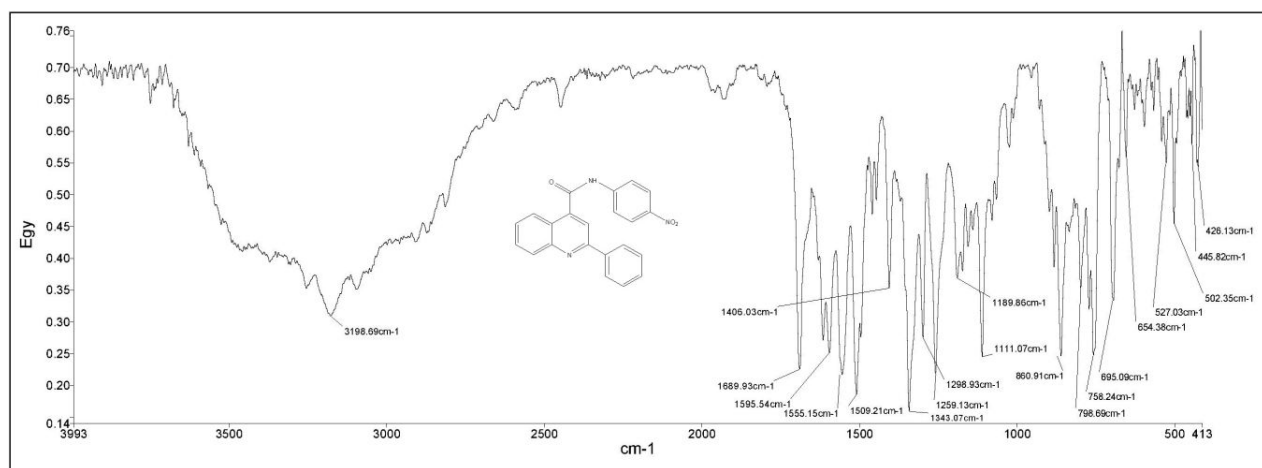
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3317, 1691, 1590, 1548, 1347, 1279, 1151, 774, 749, 690

IR of *N*-(3-nitrophenyl)-2-phenylquinoline-4-carboxamide (4i)



IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3275, 1691, 1631, 1543, 1526, 1354, 1109, 848, 752, 676

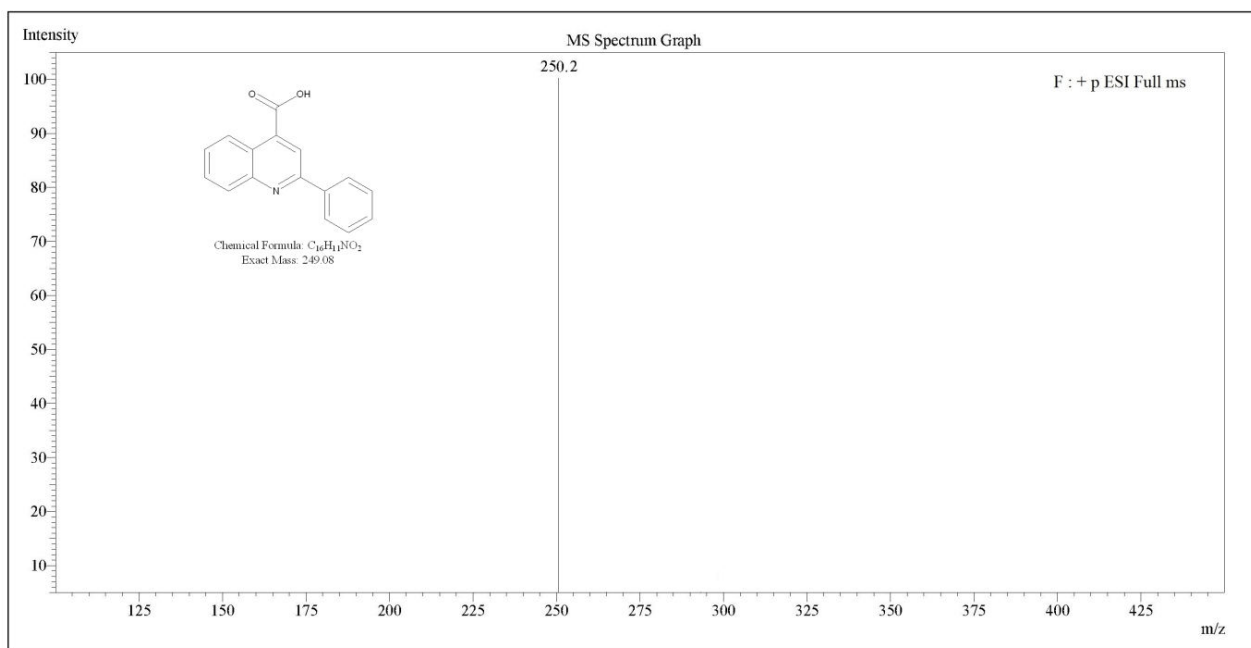
IR of *N*-(4-nitrophenyl)-2-phenylquinoline-4-carboxamide (4j)



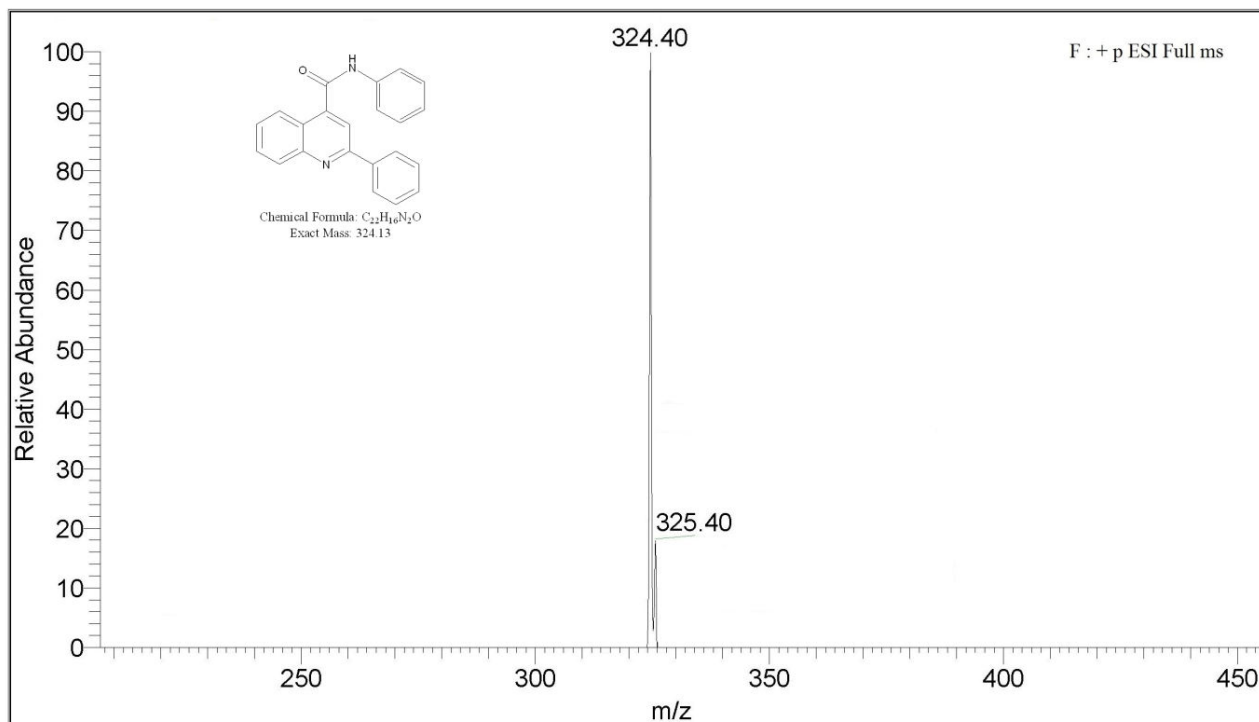
IR (KBr) $\nu_{\text{max}}/\text{cm}^{-1}$: 3198, 1689, 1595, 1555, 1343, 1259, 1189, 860, 758, 695

4. MS :

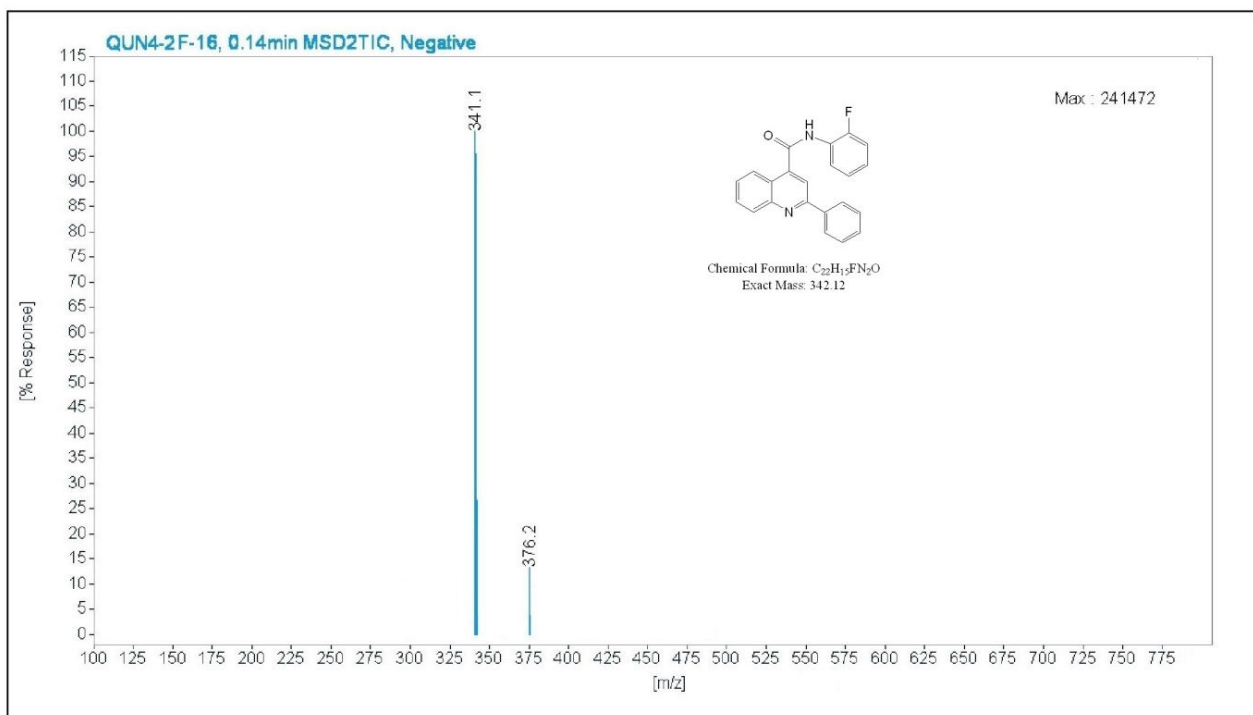
MS of 2-phenylquinoline-4-carboxylic acid (3)



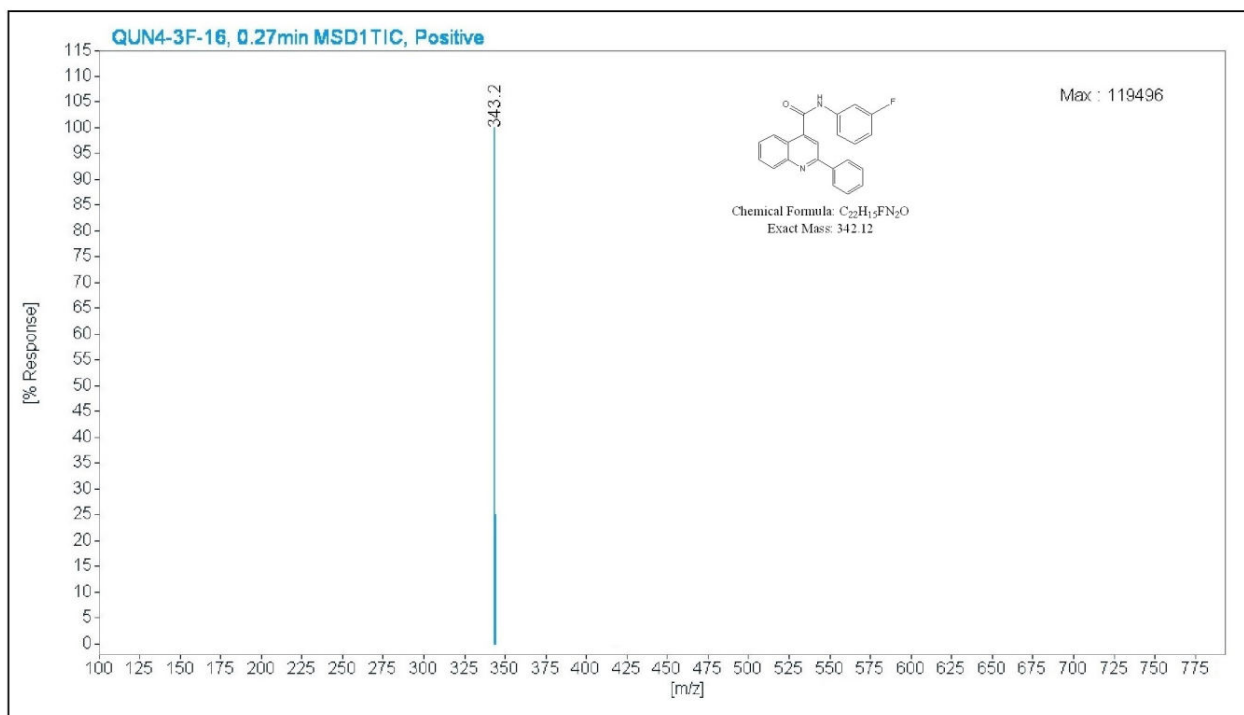
MS of Synthesis of *N,N*-2-diphenylquinoline-4-carboxamide (4a)



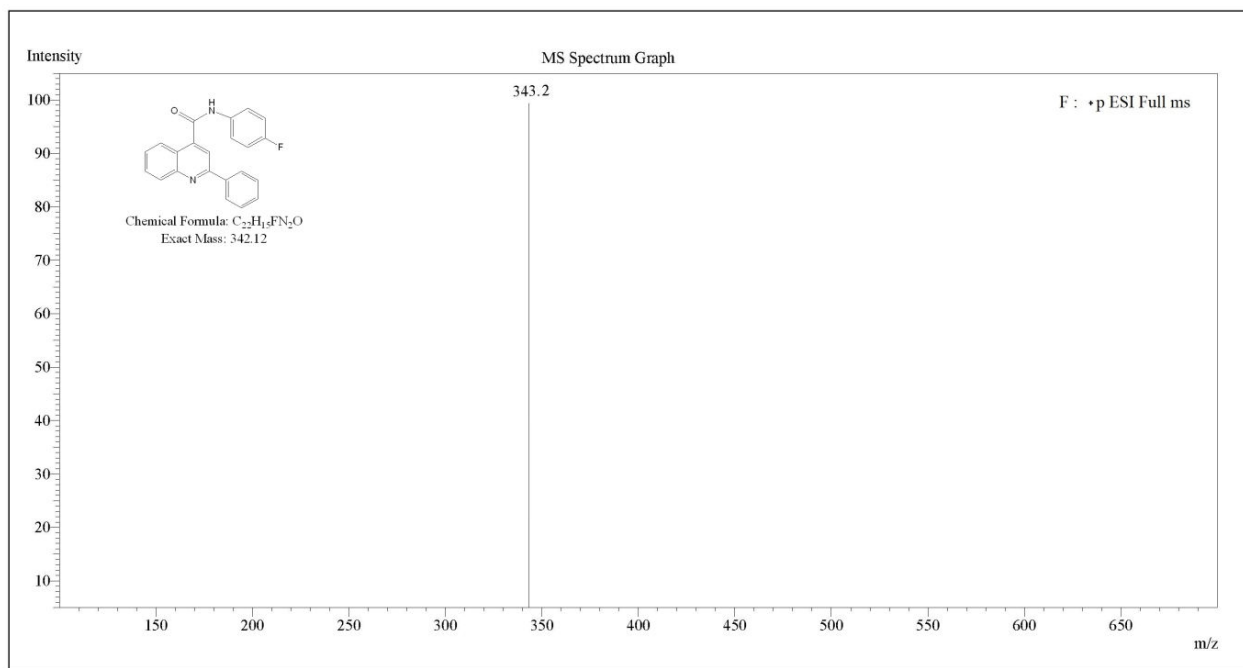
MS of *N*-(2-fluorophenyl)-2-phenylquinoline-4-carboxamide (4b)



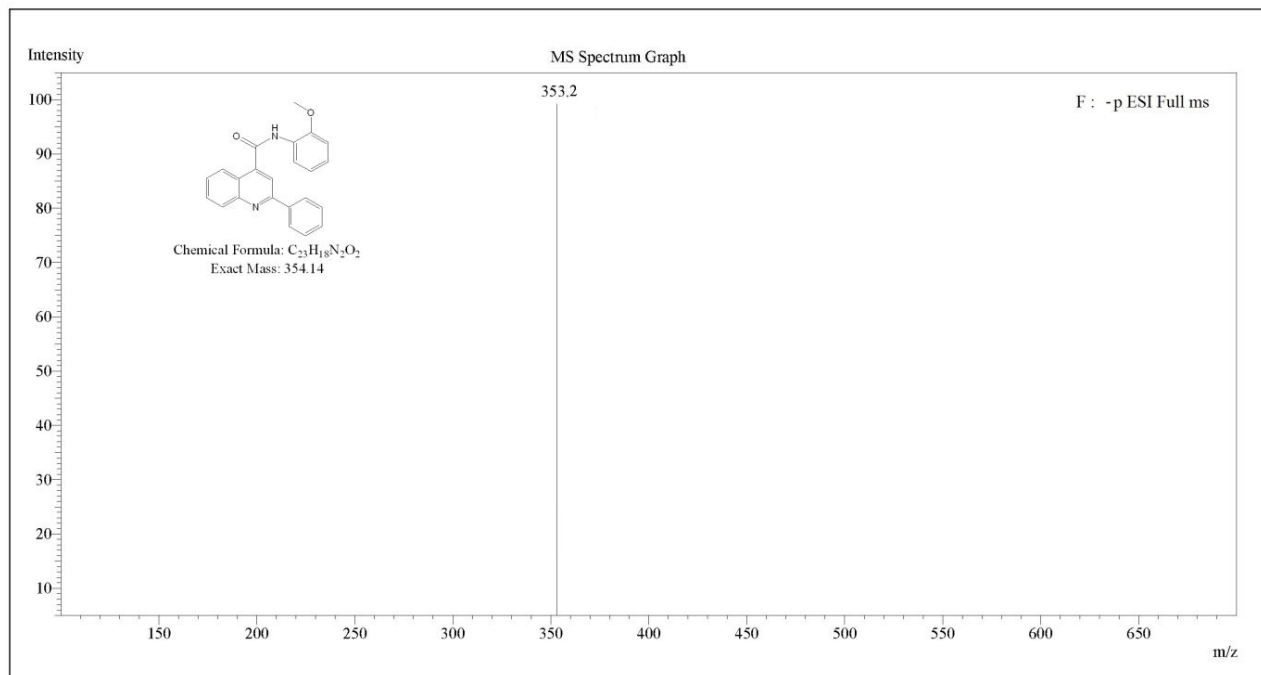
MS of *N*-(3-fluorophenyl)-2-phenylquinoline-4-carboxamide (4c)



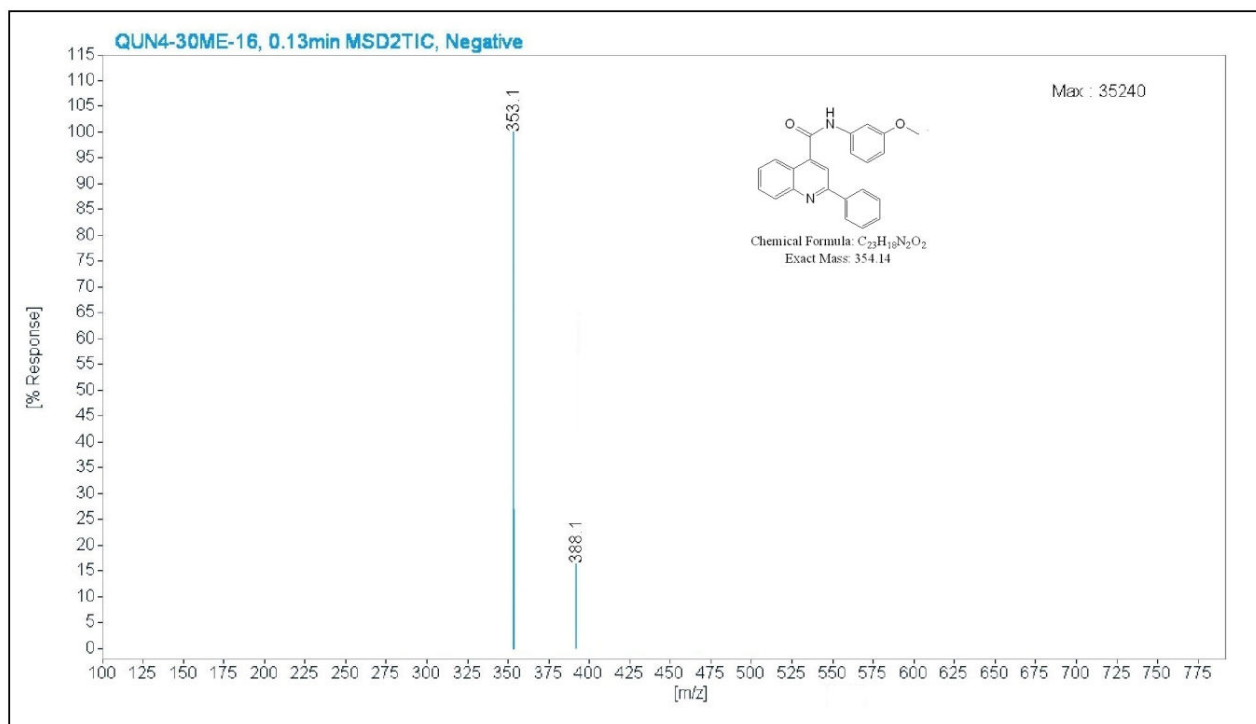
MS of *N*-(4-fluorophenyl)-2-phenylquinoline-4-carboxamide (4d)



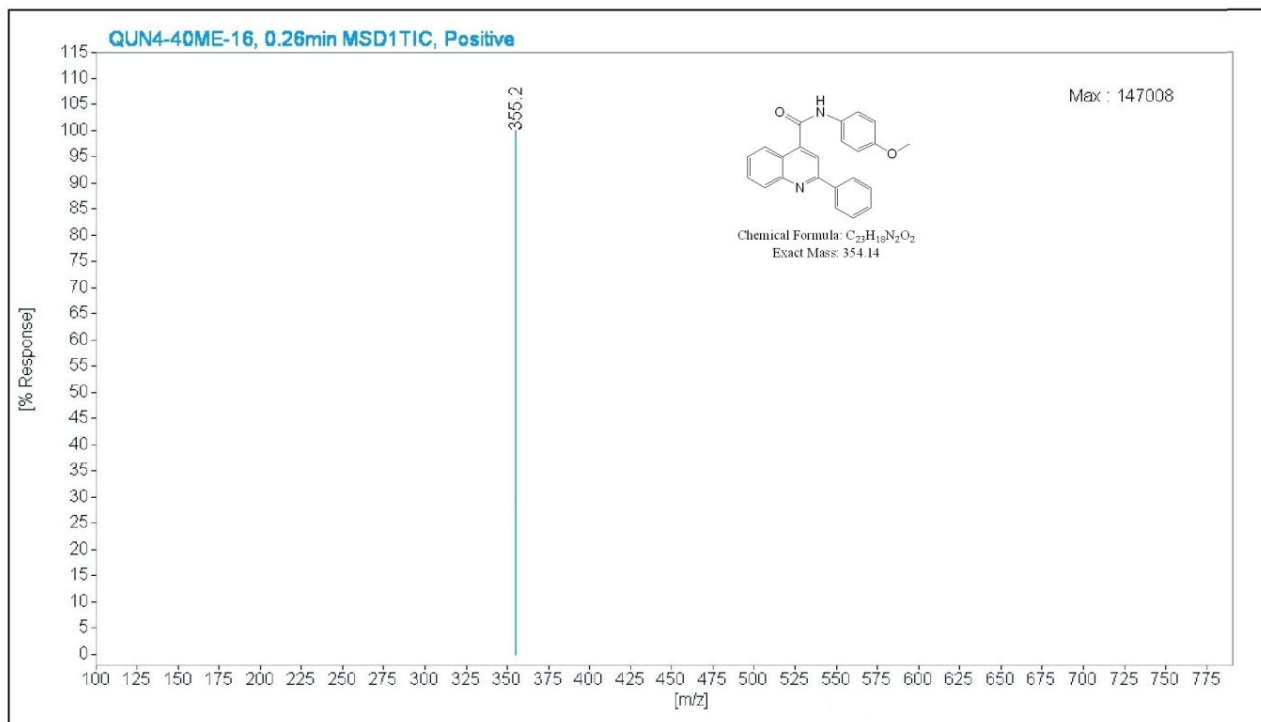
MS of *N*-(2-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4e)



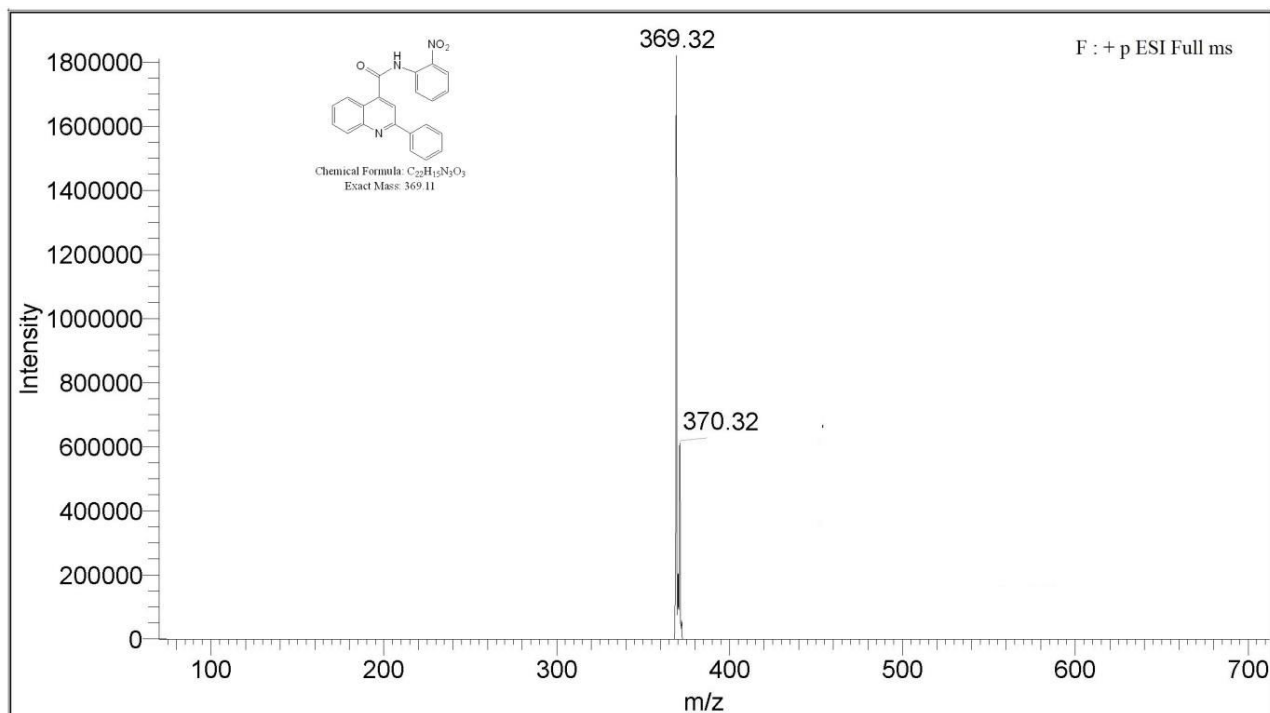
MS of *N*-(3-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4f)



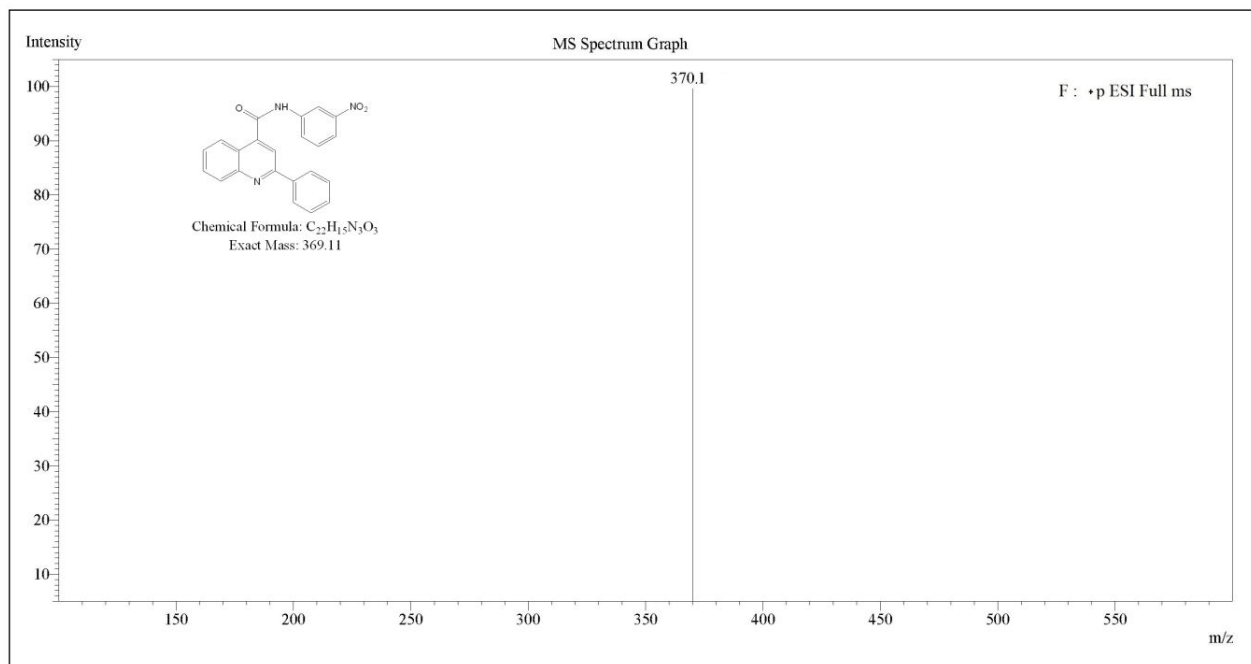
MS of *N*-(4-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4g)



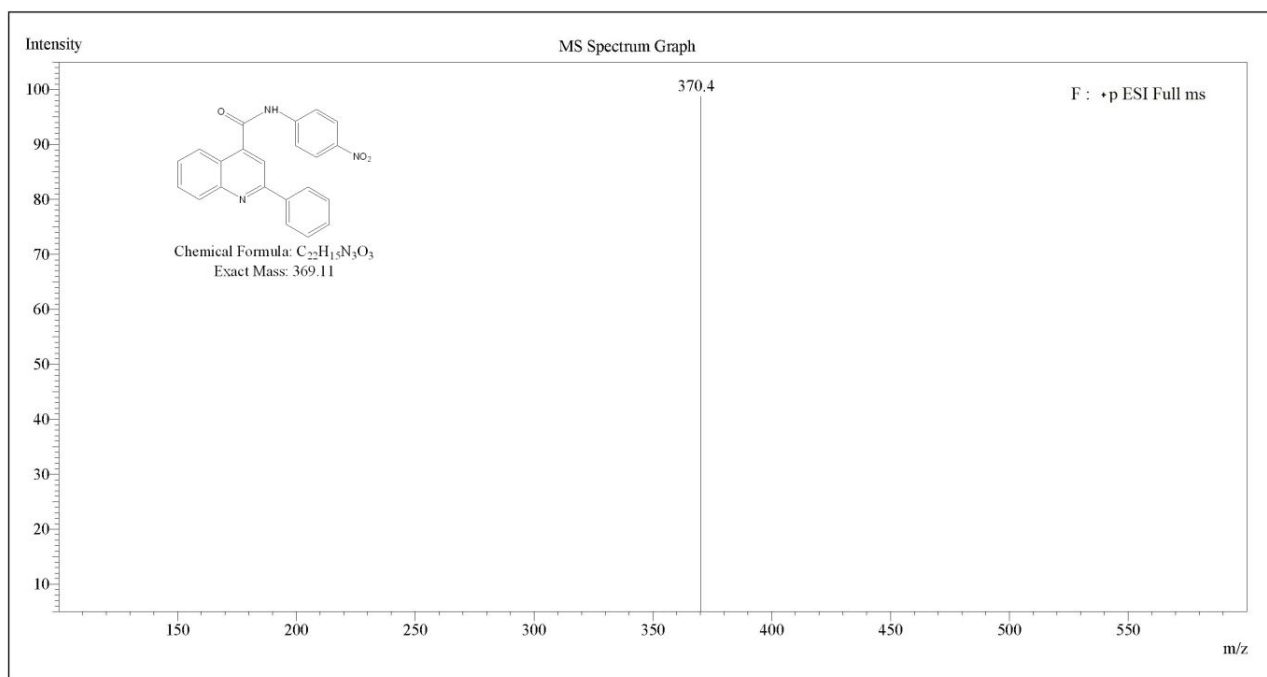
MS of *N*-(2-nitrophenyl)-2-phenylquinoline-4-carboxamide (4h)



MS of *N*-(3-nitrophenyl)-2-phenylquinoline-4-carboxamide (4i)

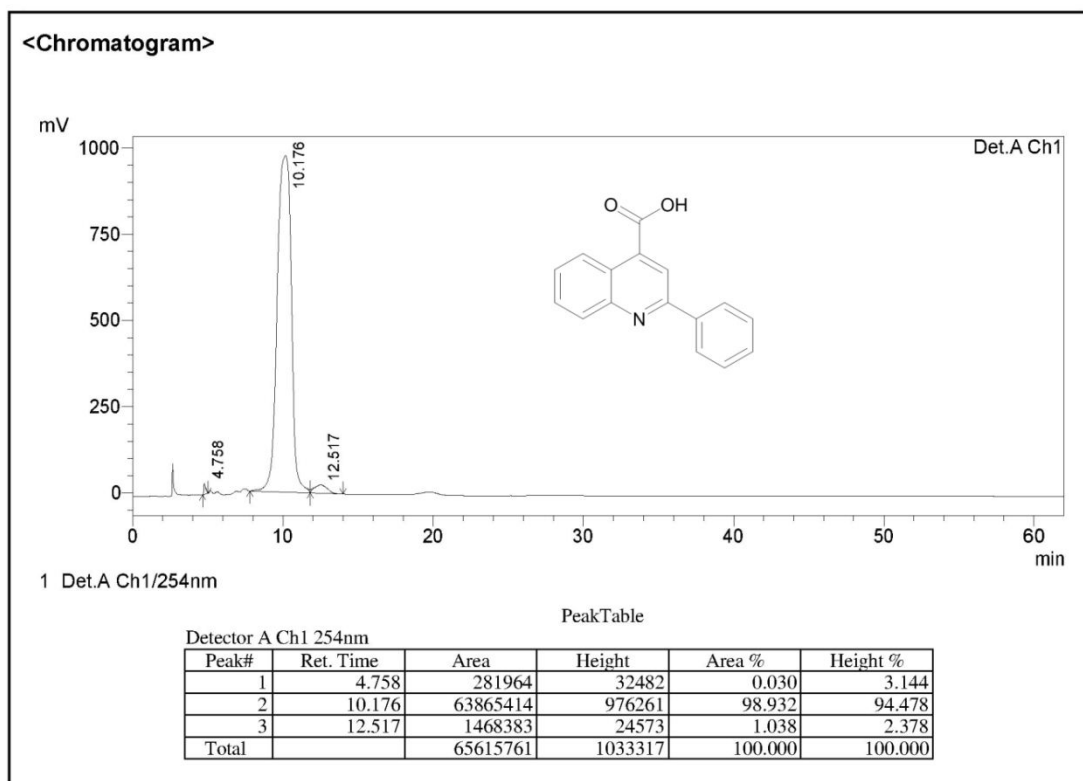


MS of N-(4-nitrophenyl)-2-phenylquinoline-4-carboxamide (4j)

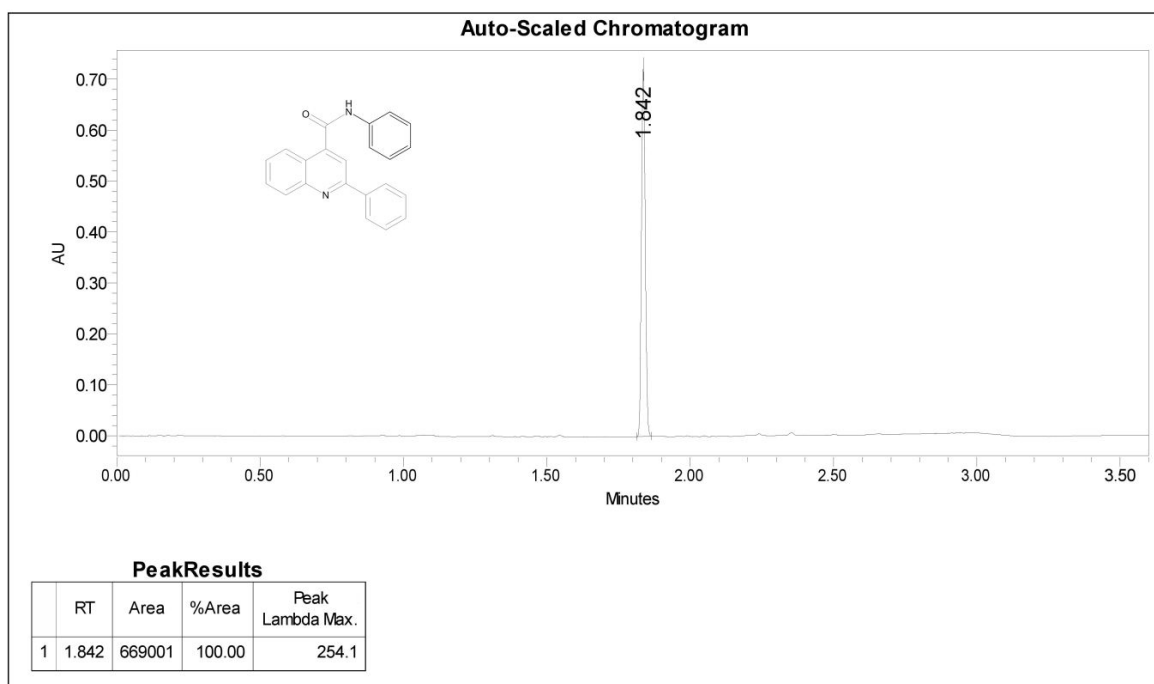


5. HPLC :

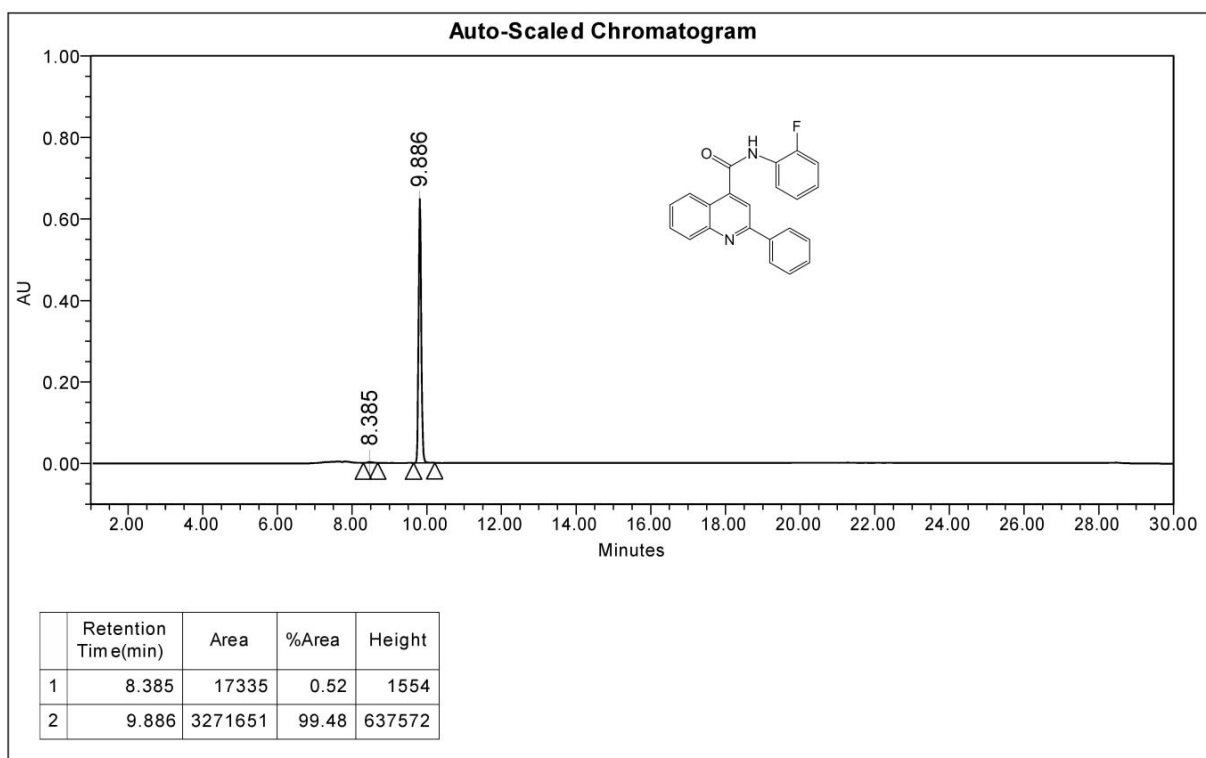
HPLC of 2-phenylquinoline-4-carboxylic acid (3)



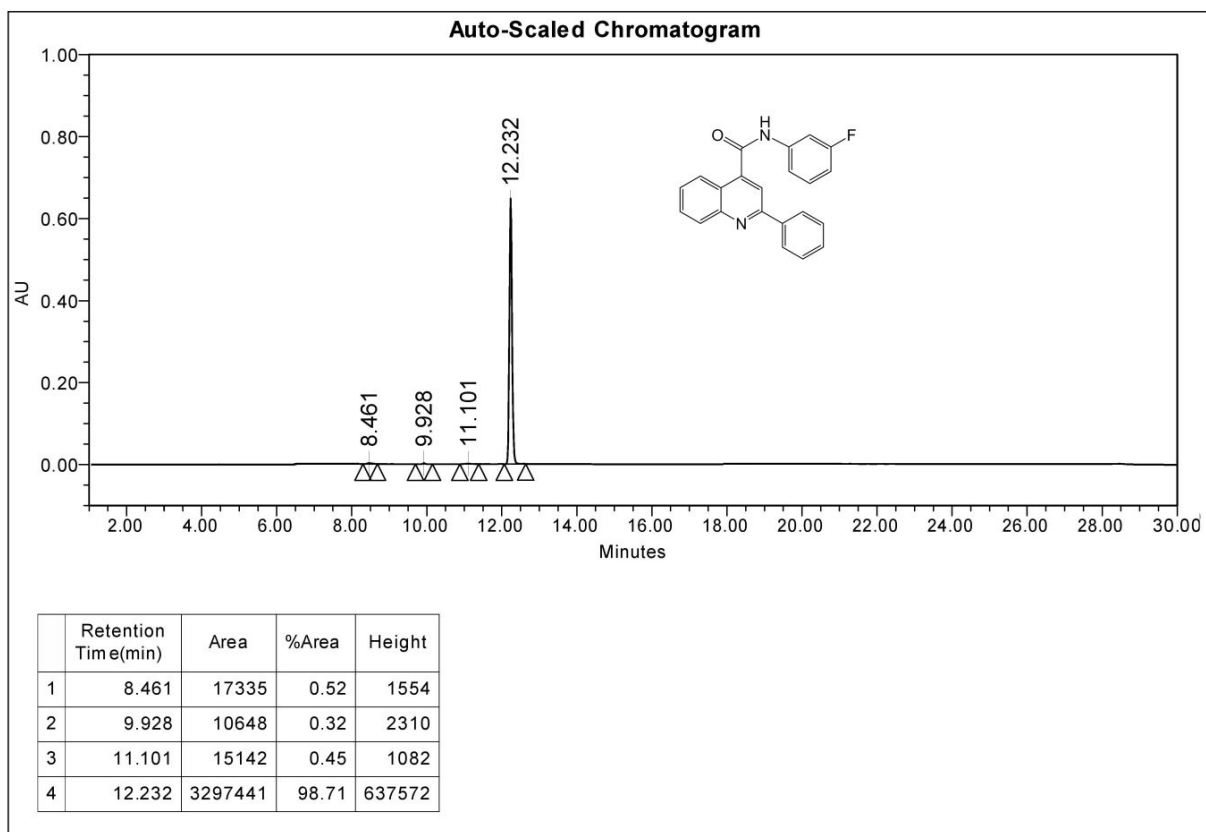
HPLC of Synthesis of N,N-2-diphenylquinoline-4-carboxamide (4a)



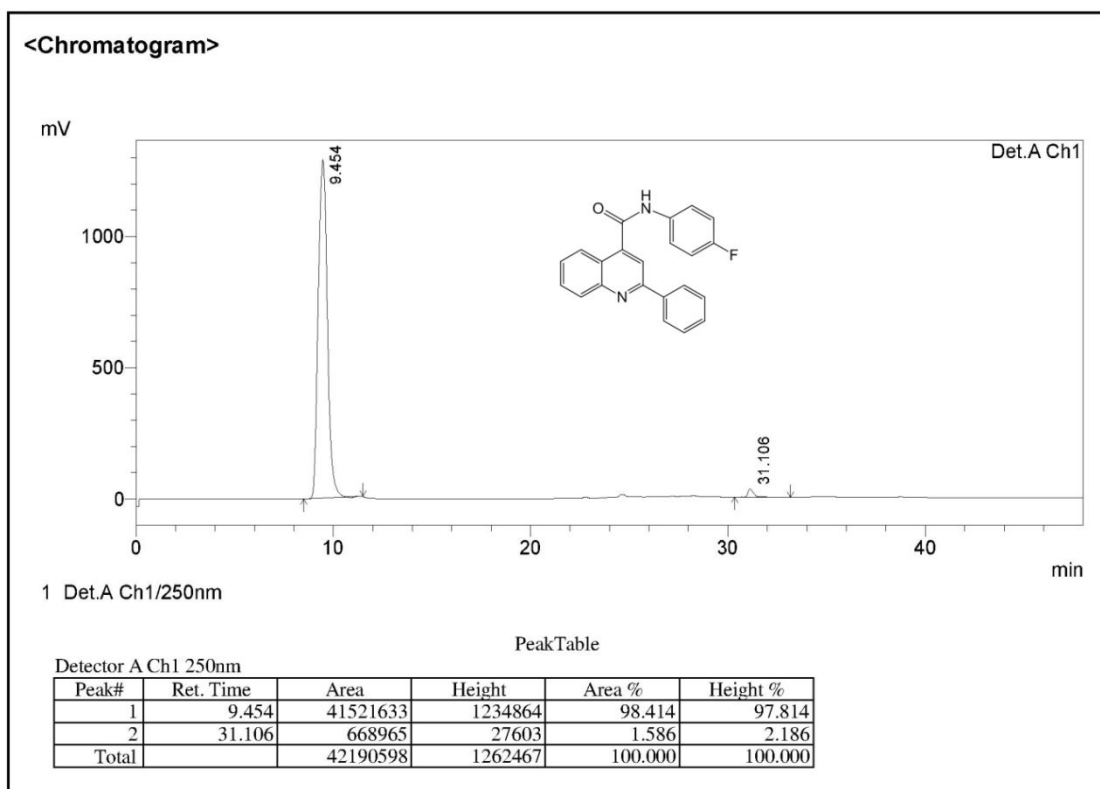
HPLC of *N*-(2-fluorophenyl)-2-phenylquinoline-4-carboxamide (**4b**)



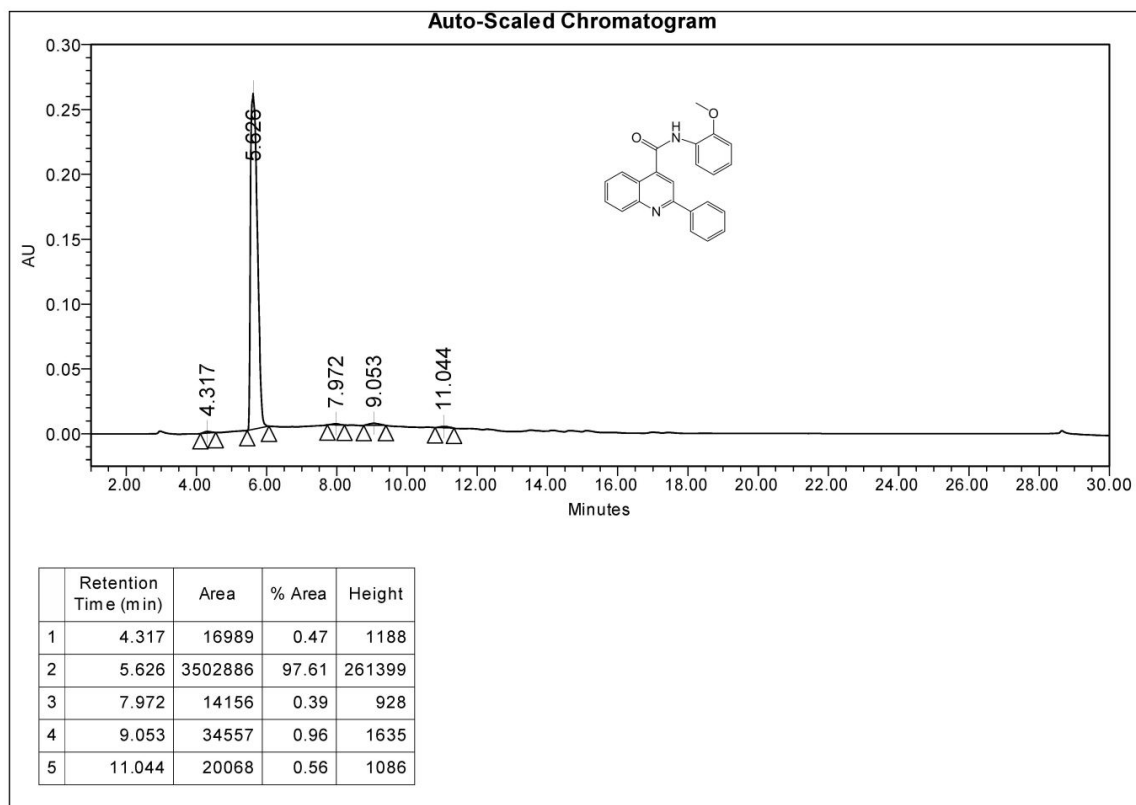
HPLC of *N*-(3-fluorophenyl)-2-phenylquinoline-4-carboxamide (**4c**)



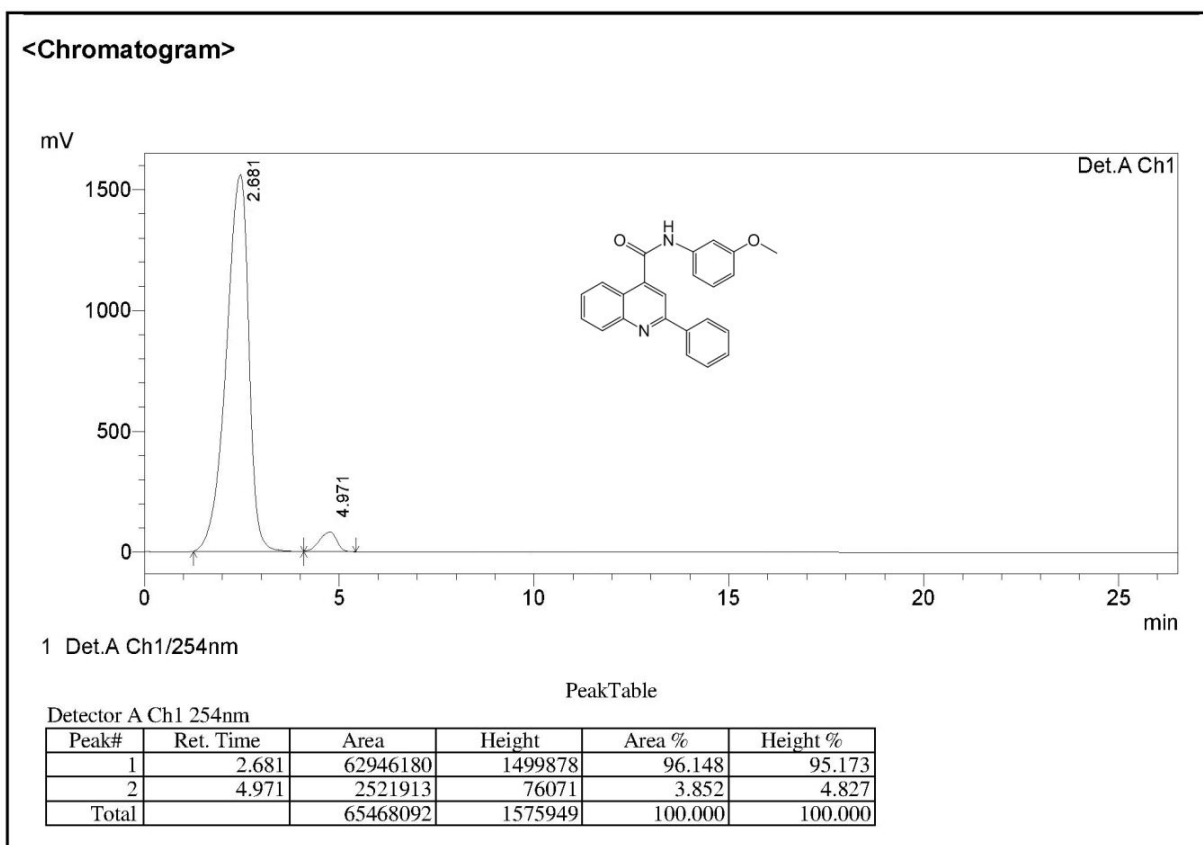
HPLC of *N*-(4-fluorophenyl)-2-phenylquinoline-4-carboxamide (4d)



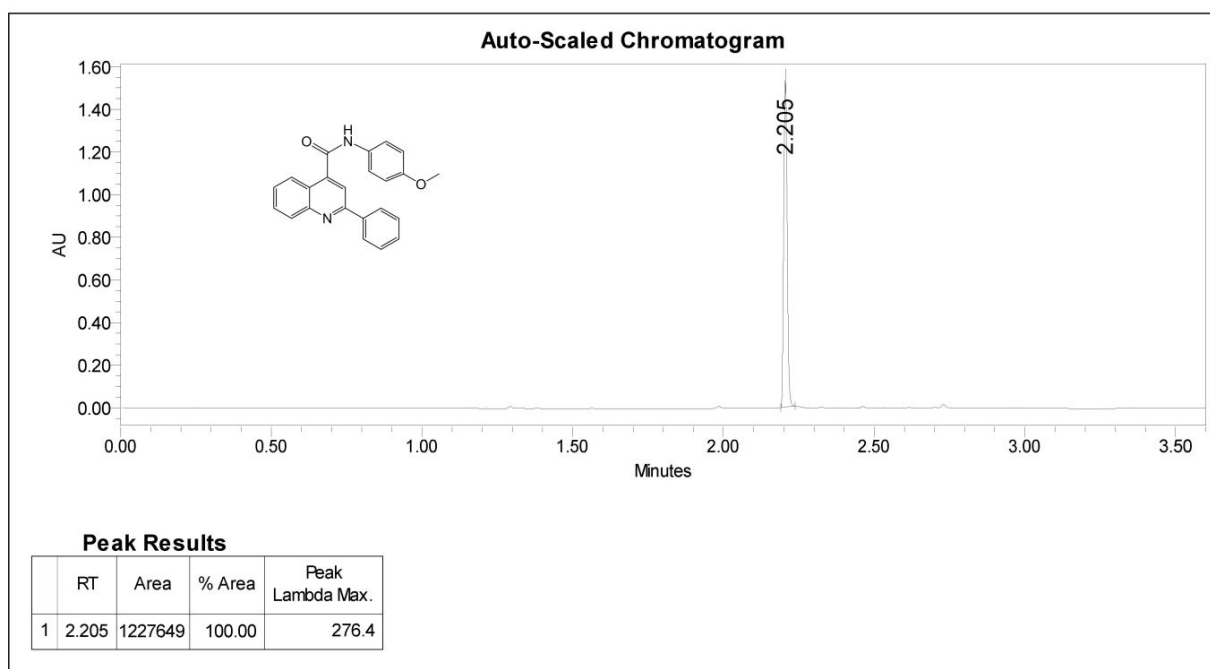
HPLC of *N*-(2-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4e)



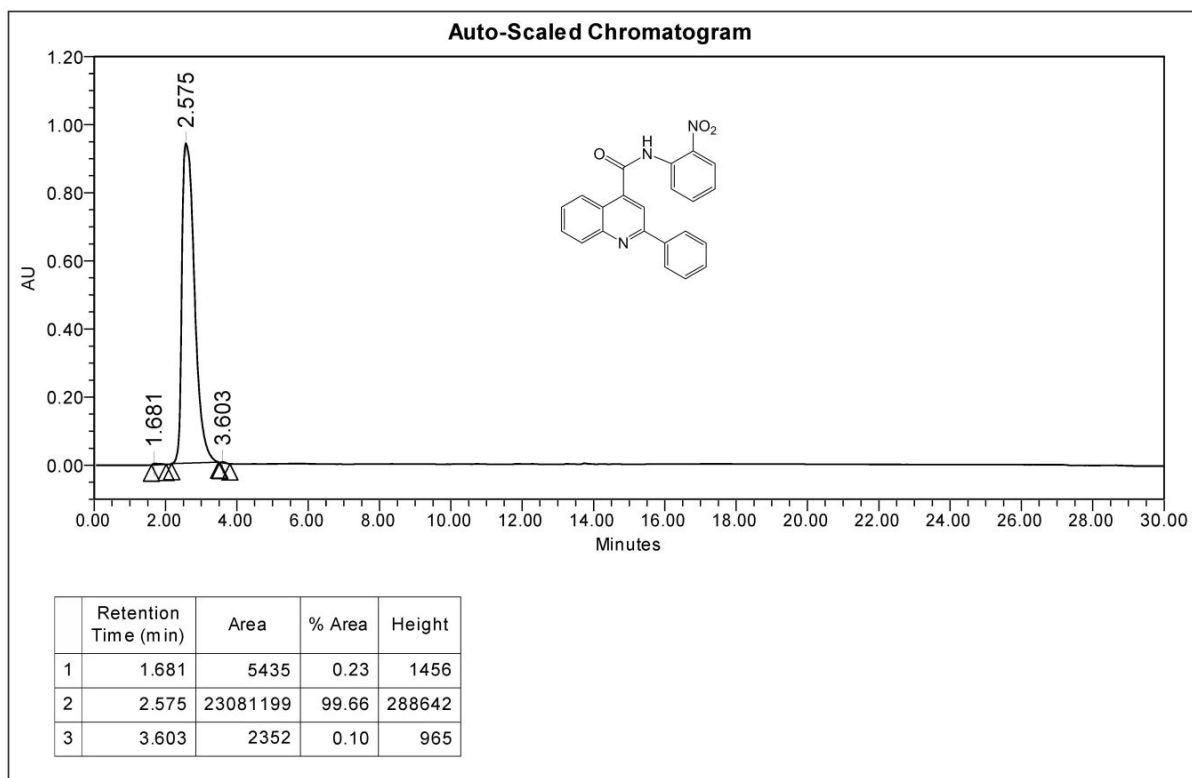
HPLC of *N*-(3-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4f)



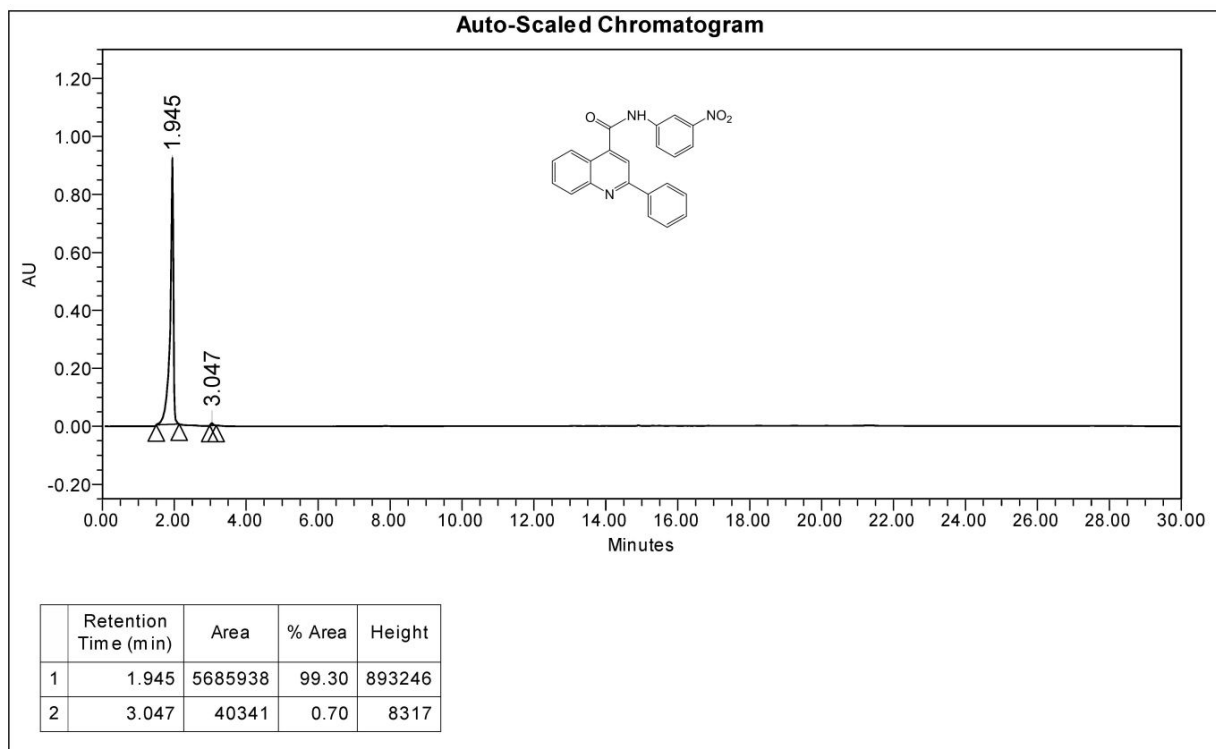
HPLC of *N*-(4-methoxyphenyl)-2-phenylquinoline-4-carboxamide (4g)



HPLC of *N*-(2-nitrophenyl)-2-phenylquinoline-4-carboxamide (4h)



HPLC of *N*-(3-nitrophenyl)-2-phenylquinoline-4-carboxamide (4i)



HPLC of *N*-(4-nitrophenyl)-2-phenylquinoline-4-carboxamide (4j)

